NUMERICAL METHODS FOR SINGULAR BOUNDARY VALUE PROBLEMS

A Thesis Submitted
In Partial Fulfilment of the Requirements
for the Degree of

DOCTOR OF PHILOSOPHY

By

KUPPUSWAMY SANTHANA RAMAN

to the

DEPARTMENT OF MATHEMATICS
INDIAN INSTITUTE OF TECHNOLOGY, KANPUR

NOVEMBER, 1984

Dedicated

To My Grandpa, Grandma

CERTIFICATE

This is to certify that the research work embodied in the thesis "Numerical methods for Singular boundary value problems" by K. Santhana Raman has been carried out under my supervision, and that this work has not been submitted elsewhere for a degree or diploma.

November - 1984

M.K. Kadalbajoo

(M.K. Kadalbajoo)
Assistant Professor
Department of Mathematics
Indian Institute of Technology
Kanpur

ACKNOWLEDGEMENTS

I wish to express my deep sense of gratitude and thanks to my supervisor Dr.M.K.Kadalbajoo for his constant encouragement, guidance and inspiring discussions throughout the completion of this thesis. My association with him has been most rewarding in my academic life.

I take this opportunity to express my gratitude to Prof.R.K.Jain, Prof.R.K.S.Rathore, Department of Maths. and Prof. S.Sadagopan, IME Department of I.I.T.,Kanpur for their help and inspiration during the research work.

I am thankful to my colleagues Muruganandam, Jain, Youvaraj, and Reddy for the valuable discussions during the preparation of the thesis.

I am also thankful to my friends Poonacha, Murali Shanta, Didi, Joy and George for their help and affection during my stay at this institute.

Thanks are also due to Sri G.L.Misra and A.K.Bhatia for their neat typing and A.N.Upadhayaya for cyclostyling.

(K.Santhana Raman)

CONTENTS

LIST OF TABLES

LIST OF PUBLICATIONS

A part of the thesis has been accepted/communicated for publication in the form of following research papers:

(1) ''Numerical solution to singular boundary value problems by invariant imbedding'', Journal of Comput. Physics, 55, no. 2, pp. 268 - 277 (1984).

(2) ''Discrete invariant imbedding method for infinite interval problems'', Accepted for publication in Appl. Math. and Computation (in press).

(3) ''Cubic spline and invariant imbedding for solving singular two point boundary value problems''. Accepted for publication in Jl. Mathematical Anal. and Application.

(4) ''Numerical solution of singular boundary value problems via Chebyshev polynomials and invariant imbedding''. Communicated to Int. Jl. of Computer Mathematics.

(5) ''Cubic spline solution of boundary value problems over infinite interval'', Communicated to Int. Jl. of Computational and Appl. Mathematics.

(6) ''Discrete invariant imbedding method for singular two point boundary value problems''. Communicated for publication.

SYNOPSIS

In many branches of Science and Engineering applications, one often encounters singular boundary value problems in ordinary differential equations, which although mathematically well conditioned, are virtually difficult to solve with analytical procedures. For solving such problems, numerical methods have received a great deal of attention in the last few years. Basically, there are two approaches to solve these problems; one is to apply directly the numerical methods to singular problems ignoring the singularity and second is to give some analytical treatment to singularity and then solve the resulting regular boundary value problem. In the former approach, one would generally need a very fine mesh especially in the vicinity of the singularity thereby increasing the computational complexity of the problem. One may also sometimes need to consider higher order methods to achieve a reasonably good accuracy. In the latter case, one expects to produce good results in view of the analytical treatment to remove the singularity in the problem. However, the ingenuity of the approach used to subtract out the singularity and then to solve the resulting regular problem, would determine the efficiency of the method.

In the present thesis, we have derived some new and efficient computational algorithms for solving singular two point boundary value problems over finite and infinite intervals.

Chapter 1 presents introduction, types of singularities, motivation with physical applications, a brief survey of the work done by earlier researchers and summary of the work done in the present thesis.

In the second chapter, a particular class of singular boundary value problems have been considered for ordinary differential equations on a finite interval, which has a singularity of the first kind. These types of problems have been discussed earlier by researchers,and arise when reducing partial differential equations by physical symmetry. The singularity is subtracted out by using the series expansion and a new boundary condition is derived in the vicinity of the singularity. A discrete invariant imbedding method has been developed to solve the resulting regular boundary value problem efficiently. The stability of the method is discussed. The proposed method is conceptually simple and easy to implement. Some test examples have been solved and the numerical results presented. A comparison of numerical results has also been made with other methods.

Chapter 3 deals with the continuous version of Invariant Imbedding method to solve the singular boundary value problems considered in Chapter 2. Again the expansion procedure has been employed to derive the new boundary condition near to singularity. Next a continuous invariant imbedding has been described to reduce the regular boundary value problem into a set of initial value problems. The Runge Kutta Fehlberg variable step size technique has been employed to integrate the stable initial value problems efficiently. Some model problems have been solved to illustrate the efficiency of the method. The continuous

Invariant Imbedding combined with variable step size initial value software have been found to be more accurate than the discrete version of Invariant Imbedding but at a slightly more cost of computational time.

The treatment given to the singularities to the problems considered in earlier chapters is based on using extended power series and thereby derive a new boundary condition near to singularity. However, in cases where there is slow convergence of the series expansion, an economized expansion may be used. In Chapter 4, we discuss Chebyshev economization near the singular point to overcome slow convergence of the series. Using the shifted Chebyshev polynomials and the Lanczos Tau method a new boundary condition near the singularity is obtained. The resulting regular boundary value problem is then treated with continuous Invariant Imbedding described in Chapter 3. Numerical results of some test examples are also included.

The attempts in earlier chapters for the removal of singularity are based on using expansion procedures in the neighbourhood of the singularity. However for some problems, it may be difficult or even not possible to obtain the series expansion near the singularity. In such cases, one may have to use a direct approach to solve singular boundary value problems. A modified fourth order finite difference method to solve a certain class of linear singular BVP's is presented in Chapter 5.

The original differential equation is modified at the singular point. The main feature of the modified difference scheme is that it leads to the tridiagonal system of equations which has been solved by discrete Invariant Imbedding method. Some model problems have been solved and the numerical results included.

The numerical solution of nonlinear singular boundary value problems has been discussed in Chapter 6. A quasi-linearization technique has been used to reduce the nonlinear problem to a sequence of linear problems. A fourth order finite difference method described in Chapter 5 has been employed to solve these problems effectively. Some model problems have been solved to demonstrate the efficiency of the method.

In Chapter 7, we have considered the infinite interval boundary value problems in ordinary differential equations. In Case I, We derive the asymptotic boundary condition to represent the infinity condition at the far end. This boundary condition has been derived such that it expresses the asymptotic behaviour of the solution as well, and converge to the actual solution of the 'infinite' problem as the length of finite interval tends to infinity. The resulting boundary value problem is treated by imbedding methods. The stability of the problem is analysed. In Case II, we have briefly included the transformation technique as an alternative method to solve these problems. For the transformed problems on a finite interval with a regular singularity at one end point of the interval, the methods discussed in earlier chapters can be applied directly.

Finally in Chapter 8, the application of cubic spline method to infinite interval problems is discussed. By reducing the infinite interval to a finite interval which is large and imposing the asymptotic boundary conditions at the far end, the two point boundary value problem on a finite interval is treated by using cubic spline approximation. The tridiagonal system resulting from the spline approximation is efficiently solved by the method of imbedding. The stability of the method is also discussed and the theory is illustrated by test examples.

In a nut-shell, the numerical methods presented in this thesis for solving singular boundary value problems over finite and infinite intervals have been shown to be efficient over other methods. Although problems with singularity at one end point have been discussed, yet one may apply these methods to problems with interior regular singularities or two regular singular end points. The invariant imbedding methods is conceptually simple, easy to implement, and has the properties of solving boundary value problems subject to different boundary conditions without extra computational effort.

Model problems have been solved and numerical results presented in respective chapters. The numerical results presented, in this thesis have been computed on DEC-1090 system in single precision arithmetic.

INTRODUCTION

In the recent past, methods for numerically solving two point boundary value problems for differential equation have been extensively studied by several researchers. A number of methods like Shooting Methods [17 , 55 , 78] , Finite difference methods [27 , 55 , 57 , 63 , 67 , 81], Collocation Methods [1, 18, 82] and Invariant imbedding methods [6 , 11 , 13 , 15 , 19 , 58 , 69-71, 77 , 79 , 85-90] have been reported in the literature for solving these problems. However little effort seems to have been devoted to the solution of Singular two point boundary value problems in ordinary differential equations. Difficulty arises in solving Singular boundary value problem due to the fact that the coefficient functions in the differential equation are not analytic. When the analytical methods fail to produce the solution of Singular boundary value problem (SBVP), one then should try to ascertain the approximate nature of the solution. Therefore, it is very useful to develop numerical methods to obtain approximate solution to hard problems like SBVP. Such attempts may prove to be useful in many practical situations where, analytical solutions are difficult to obtain. The purpose of this thesis is to devise and develop efficient computational methods for solving singular boundary value problems over finite and infinite Intervals. It would be pertinent here to first give the classification of singularities and their occurrence in practical applications.

1.1 Types of Singularities

We begin the process of local analysis by classifying the singularities. Singularities can be of two kinds : (i) Singularity of the first kind which is also known as Regular Singularity, and (ii) Singularity of the second kind, which is sometimes refered to as essential singularity. We classify a point x_o, which may be an Ordinary point, a regular singular point or an irregular singular point of a differential equation as follows :

Suppose we consider a second order linear differential equation of the form,

$$f_o(x)y''(x)+f_1(x)y'(x)+f_2(x)y(x) = f_3(x), \quad x \in [x_o, b] \qquad (1.1)$$

where $f_o(x)$, $f_1(x)$ and $f_2(x)$ are analytic in the neighbourhood of some point $x = x_o$(say), then $x = x_o$ is said to be an <u>Ordinary point</u> in the sense that the solution of (1.1) can be represented by a Taylor series in powers of $(x-x_o)$. If for some point $x = x_o$, $f_o(x_o) = 0$ and $f_1(x_o) \neq 0$, then x_o is called a <u>Singular point</u> of the equation (1.1). In such a case rewriting Eqn. (1.1) in the form

$$y''(x)+F_1(x)y'(x)+F_2(x)y(x) = F_3(x) \qquad (1.2)$$

where $F_i(x) = \dfrac{f_i(x)}{f_o(x)}$, $i = 1,2$, we see that the coefficients $F_1(x)$ and $F_2(x)$ fail to be analytic at $x = x_o$.

The point $x = x_0$ is said to be a Regular Singular point of (1.2) if $(x-x_0)F_1(x)$ and $(x-x_0)^2F_2(x)$ are analytic at $x = x_0$. A solution of (1.2) may be analytic at a regular singular point. If it is not analytic its singularities must be either a pole or an algebraic or logarithmic branch point. It is pointed that there is always one solution of the form

$$y(x) = (x-x_0)^{\alpha} A(x)$$

where α is a number called the indicial exponent and $A(x)$ is a function which is analytic at x_0 and which has a Taylor series whose **radius** of convergence is atleast as large as the distance to the nearest singularity of the coefficient functions.

The point $x = x_0$ $(x_0 \neq \infty)$ is called an Irregular Singular point of (1.2) if it is neither an ordinary point nor a regular singular point. There is no comprehensive theory of irregular singular points, we can say that at an irregular point, all functions exhibit as essential singularity, often in combination with a pole or an algebraic or logarithmic branch point.

Often it is of interest to investigate solutions of the form (1.2) for large values of x, say $x = \infty$. A simple way of doing this is to make use of the substitution $x = \frac{1}{t}$ in (1.2), and study the solutions of the resulting equation near $t = 0$. Then, for example, the results on analytic equations and equations with a regular singular point $t = 0$ can be applied. Using the substitution $x = \frac{1}{t}$ Eqn. (1.2) reduces to the form

$$t^2y'' + \left(2 - \frac{\tilde{F}_1(t)}{t}\right) ty' + \frac{\tilde{F}_2(t)}{t^2} y = \frac{\tilde{F}_3(t)}{t^2} \tag{1.3}$$

where $\tilde{F}_1(t) = F_1(\frac{1}{t})$, $\tilde{F}_2(t) = F_2(\frac{1}{t})$ and $\tilde{F}_3(t) = F_3(\frac{1}{t})$. We say that infinity is a regular singular point for (1.2) if the Eqn. (1.3) has the origin $t = 0$ as a regular singular point. If $t = 0$ is not a regular singular point, then infinity is said to be an irregular singular point.

The simplest example of an equation with a regular singular point at infinity is the Euler's equation. viz.

$$a^2y'' + axy' + by = 0$$

where a,b are constants. This equation has the origin and infinity as regular singular points.

1.2 Motivation and Physical Problems :

Singular boundary value problems for ordinary differential equations arise very frequently in several areas of science and Engineering. For example, consider the following boundary value problem

$$\frac{d^2T}{dx^2} + \frac{p}{x}\frac{dT}{dx} + f(T) = 0, \quad \frac{dT(0)}{dx} = 0, \quad T(1) = 1 \tag{1.4}$$

which results from an analysis of heat conduction through a solid with heat generation. The function $f(T)$ represents the heat generation within the solid; this, in general, is a function of the local temperature T. The constant p is equal to 0, 1 or 2 depending on whether the solid is a plate, a cylinder or a sphere. In a simple case when $p = 0$, the solid

is a flat plate with constant heat generation and $f(T) = q/K$, where K is the heat conductivity and q is a heat generation per unit volume. Eqn. (1.4) then becomes

$$\frac{d^2T}{dx^2} = \frac{q}{K} = 0, \quad \frac{dT(0)}{dx} = 0, \quad T(1) = 1$$

which is a linear differential equation with constant coefficients. Thus, we arrive at a two point boundary value problem which has been solved efficiently by many authors.

Consider next the case in which the solid is a cylindrical rod and the heat generation is linearly proportional to the temperature T. Then $f(T) = \beta^2 T$ with $p = 1$, and Eqn. (1.4) becomes

$$\frac{d^2T}{dx^2} + \frac{1}{x}\frac{dT}{dx} + \beta^2 T = 0 \quad , \quad \frac{dT(0)}{dx} = 0, \quad d(1) = 1 \qquad (1.5)$$

which is a linear differential equation with variable coefficients. For these types of problems the solution becomes complicated due to the singularity arising in the differential equation. One then needs to take extra care to solve these problems. Similarly when $p = 2$ and the heat generation is written as $f(T) = \alpha e^T$, where α is a constant, Eqn.(1.4) becomes

$$\frac{d^2T}{dx^2} + \frac{2}{x}\frac{dT}{dx} + \alpha e^T = 0, \quad \frac{dT(0)}{dx} = 0, \quad T(1) = 1 \qquad (1.6)$$

This problem becomes a nonlinear boundary value problem due to the nonlinearity of the heat generation term. For such types

of problems, the numerical methods seem to be the only choice for their solution.

To quote a few more examples of practical importance in different areas, we have :

i) In Astronomy : The equilibrium of isothermal gas spheres can be described by

$$y''(x) + \frac{2}{x} y'(x) + (y(x))^5 = 0$$
$$y'(0) = 0 \; ; \; y(1) = \frac{1}{2}\sqrt{3} \qquad (1.7)$$

This problem is of the form (1.4).

ii) In Chemistry : The formulation of heat and mass transfer within porous catalyst particle leads to [48]

$$y''(x) + \frac{a}{x} y'(x) = \Phi^2 \; y(x) \; \exp\left[\frac{\gamma\beta(1-y(x))}{1+\beta(1-y(x))}\right]$$
$$y'(0) = 0; \quad y(1) = 1 \qquad (1.8)$$

where

y : dimensionless concentration,

a : Structure of Catalyst particle, $a = 2$ spherical,

β, γ, Φ : Chemical constants.

iii) Thomas-Fermi Model : The Thomas-Fermi model in atomic physics describes the charge concentration $y(x)$ of electrons in an ion :

$$y''(x) = x^{-\frac{1}{2}} (y(x))^{1/2}$$

$$y(0) = 1 \; ; \quad y(b) = 0. \tag{1.9}$$

iv) The Ginzburg-Landau Equations : A problem in superconductivity to find cylindrically symmetric solutions of the Ginzburg-Landau equations with radius r, fluxoid quantum number n = 1, and Ginzburg-Landau parameter K = 1 leads to

$$L\,[f(x)] = K^2\, f(x)\ (f^2(x) - 1 + a^2(x) - \frac{2}{Kx}\, a(x))$$

$$L\,[a(x)] = f^2(x)\ (a(x) - \frac{1}{Kx}) \tag{1.10}$$

$$a(0) = 0 \; ; \quad a(r) = R$$

$$0 \leq x \leq r$$

$$f(0) = 0 \; ; \; f'(r) = 0$$

where $f(x)$: order parameter,

$a(x)$: vector potential,

R : free parameter,

$r = 10$

and $L\,[\cdot] = \frac{d^2(\cdot)}{dx^2} + \frac{1}{x}\frac{d(\cdot)}{dx} - \frac{1}{x}(\cdot)$

v) Thin Shallow Spherical Shell : The elastic stability of thin shallow spherical shells subject to uniform pressure is described by [67,91]

$$f''(x) = -\mu^2\, g(x) - 2\gamma + f(x)\; g(x) - \frac{3}{x}\, f'(x)$$

$$g''(x) = \mu^2 f(x) - \frac{1}{2} f^2(x) - \frac{3}{x} g'(x)$$

$$f'(0) = g'(0) = 0, \qquad (1.11)$$

$$f(1) = 0, \; g'(1) + (1-\nu)\, g(1) = 0 \text{ clamped edge condition,}$$

where

x : normalized polar angle

$f(x)$: normalized angular deflection

$g(x)$: normalized stress

γ : load parameter

μ^2 : geometry of the shell

$\nu = \frac{1}{3}$ (Poisson's ratio).

A few notable examples of boundary value problems over infinite intervals are the Von Karman Swirling flows [61], a Combined forced and free convection flow over a horizontal plate [84], an eigen value problem for the Schrödinger equation [62], Falker-Skan equation in boundary layer theory [67], Unsteady flow of power-law fluids [67], Flow through a porous medium [67] and several others.

In the next section, we give the survey of literature on regular singular boundary value problems over finite intervals. In section 1.4, the work on infinite interval boundary value problems, done by several researchers is given. The work, done on boundary value problems with essential singularity is given in section 1.5. Finally, a short summary of the work done in the present thesis is included.

1.3 Singular boundary value problems with a Regular singularity :

For the last two decades, considerable number of methods have been discussed for solving Singular boundary value problems in ordinary differential equation with a singularity of first kind on a finite interval. These methods have been developed either to treat singular boundary value problems directly or to first give local treatment to singularity and then solve the resulting regular problem. We begin with a method based on Finite difference analysis. A numerical method for generalized axially symmetric potential of a function $u(x,y)$ described by

$$L_k[u] = \Delta u + \frac{k}{y}\frac{\partial u}{\partial y} = 0 \qquad (1.12)$$

satisfying certain boundary conditions was first studied by Parter [72]. However this particular type of partial differential equation can be reduced to the differential equation of the form

$$\frac{d^2u}{dx^2} + \frac{k}{x}\frac{du}{dx} - qu = 0, \quad |k| < 1, \; q > 0 \qquad (1.13)$$

by separation of variables for the equation (1.12) in a rectangle. Jamet [50] considered a linear ordinary differential equation of the second order

$$Lu = \frac{d^2u}{dx^2} + f(x)\frac{du}{dx} - g(x)u = H(x) \qquad (1.14)$$

where

$f(x) \ \varepsilon \ C(0,1]$

$f(x) \to \infty \quad \text{as } x \to 0$

$g(x), \ H(x) \ \varepsilon \ C[0,1]$

$g(x) \geq 0.$

According to rate of growth of f(x) near the origin, the problem to be posed may be a two point boundary value problem or one point boundary value problem. The author studied the application of three point finite difference approximation with a uniform mesh h and showed that the error is $O(h^{1-\sigma})$ when $f(x) < \frac{\sigma}{x}$, for x small, σ a constant with $0 < \sigma < 1$. The existance and uniqueness of the solution alongwith the convergence of certain finite difference schemes have been discussed.

In another work, Ciarlet [24] has considered a nonlinear two point boundary value problem whose coefficients have a singularity of first kind. Based on Ritz-Galerkin's piecewise linear approximation, the error in the uniform norm of $O(h^{2-\sigma})$ has been given. This work is the extension of the author's work for a nonlinear two point boundary value problem [23].

Application of finite difference method to singular problems has also been discussed by Gustaffsson [47] for a scalar case. Due to effect of singularity, if a difference approximation is applied on the whole interval, the convergence rate will be very poor. To improve upon the convergence, a series solution

can be represented on a subinterval near the singularity, to obtain a regular boundary value problem on the remaining interval. A centered rth order approximation is used to get a convergence rate $O(h^r)$ on the whole interval, provided the series solutions are calculated with rth order accuracy.

An approach via generalized projection method involving appropriate generalized spline functions which prove the converge faster than the usual finite difference scheme has been used by Natterer [68] for the numerical treatment of first order system of ordinary differential equation with a regular singularity. The author considers the aoproximation of the solution of singular boundary value problems such as

$$y'' + x^{-1}Uy + Wy = f, \qquad 0 < x < 1, \tag{1.15}$$

where y is a vector in R^n, U is a constant matrix and where the matrix W and the vector f depend continuously on x. In fact more general forms are considered where a similar singularity is allowed at the other end point. With the differential equation (1.15) are associated appropriate boundary conditions, the form of which depends upon the matrix U. After a careful study of the continuous problem, a projection method using generalized vector valued splines is described. The main result is that, with special choices of non-uniform meshes the convergence is the same as in nonsingular case up to a logarithmic factor.

For a second order linear differential equation with a regular singular point, Cohen and Jones [26] have applied an economized chebyshev expansion on the interval (0,1] instead of the series expansion. A second order finite difference method with deferred correction has been applied outside the range of economized expansion.

The studies of more general linear and nonlinear singular boundary value problems have been made by Russel and Shampine [83]. The aim of the study is to compare the applicability of the Finite difference, Collocation and Patch bases procedures and the ease and effectiveness of their numerical computation. The collocation with piecewise polynomial functions in different subintervals with a particular choice of collocation points for nonlinear two point boundary value problems has been described. A three point finite difference methods along the lines of Jamet [50] and Rose [81] has been used in their finite difference analysis. Patch bases method discussed earlier by Rose [81] has been extended to Singular boundary value problems. The authors feel that in many circumstances one ought to use the traditional finite difference methods. The collocation results presume the mesh space h is sufficiently small, to even guarantee the approximate solution exist. They emphasized one might use the collocation if higher order procedures of uniform mesh or if one has complicated boundary conditions.

F.R. de Hoog and Weiss [29] have studied the solution for a first order system with a singularity of first kind. The application of some standard finite difference schemes (Box scheme and Euler's scheme) for the problem

$$y'(t) - \frac{M}{t}\, y(t) = f(t,y), \qquad 0 \le t \le 1$$

with $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (1.16)

$$b(y(0), y(1)) = 0$$

and the linear eigen value problem

$$y'(t) - \frac{M}{t}\, y(t) - A(t)y(t) = \lambda G(t) y, \quad 0 \le t \le 1$$

with $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (1.17)

$$b(y(0),\ y(1)) = 0$$

with necessary boundary conditions, has been investigated. The author's restrict their attention to the case when the solutions to these problems are continuous on $[0,1]$ and differentiable on $(0,1]$. The main aim of this work is to derive the most general boundary condition, which yields a Fredholm alternative for the problems. Under natural assumptions the finite difference schemes are shown to converge and have the usual convergence (up to possible logarithmic term for box scheme) provided y, f and b are sufficiently smooth. The asymptotic expansion of the error is then examined for a number of specific cases and shown that the Keller's Box scheme has an $O(h^2)$ expansion for many important problems.

In a recent work, Reddien [73] studied a collocation method for the numerical solution of singular boundary value problems. These methods were developed by considering certain projection on to a finite dimensional linear spaces of singular polynomial splines. The purpose of this note is to enhance the applicability of the methods by showing that the class of singular splines used in [74] possess convenient local support bases which are of considerable advantage in the actual computations.

A detailed description of a shooting algorithm based on a Taylor series method is discussed by Rentrop [75] for the solution of a two point boundary value problem of the form

$$\begin{aligned} & y' = f(t,y), \\ & y : [a,b] \to R^N ; \; f : [a,b] \times R^N \to R^N \qquad (1.18) \\ & r(y(a),y(b)) = 0; \; r : R^N \times R^N \to R^N \end{aligned}$$

The author extends this work to singular problem. The algorithm computes a Taylor series expansions in a small interval in order to kill the numerical singularity and a multiple shooting technique is used to solve the problem on the remaining interval. The reliability of the method is demonstrated by solving the Ginzburg-Landau equations [76] arising in the theory of superconductivity.

A numerical method for linear systems of first order equations with a regular singular point at one end point has been

given by Brabston and Keller [16]. A class of problems considered for their analysis is,

$$
\begin{aligned}
Ly(t) &\equiv y'(t) - A(t)y(t) = f(t), \quad 0 < t \leq 1 ; \\
\mathbb{B}y(t) &= \lim_{t \to 0} [B_o(t)y(t) + B_1 y(t) - b(t)] = 0 ; \qquad (1.19) \\
A(t) &\equiv t^{-1}R + A_o(t).
\end{aligned}
$$

where $y(t)$, $f(t)$, $b(t)$ are n vectors while $R, A_o(t), B_o(t), B_1$ are nxn matrices. The author's assumed $A_o(t)$ analytic on $(0,\delta_o]$ and sufficiently smooth on $(0,1]$. Similarly $B_o(t)$, $f(t)$ and $b(t)$ are smooth on $(0,1]$ but may be singular at $t = 0$. The standard procedure of expanding about the singularity to get a nonsingular problem over a reduced interval is justified in some detail. The truncated regular two point problem is approximated by a stable rth order difference scheme (or centered Euler) as presented in [57]. The net is chosen to be uniform. The results computed are of $O(h^2)$ accurate approximations. The author's also used Richardson extrapolation to get $O(h^4)$ approximations.

Jesperson [51] studied the application of Ritz-Galerkin method for singular boundary value problems of the type arising when Poisson's equation $-\Delta u = f$ is encountered on a domain with cylindrical or spherical symmetry and is reduced to a one dimensional problem. The idea of the method is to derive a periori L_2 and L_∞ norm estimates for the error. The difficulty is that these norms are not natural norms for the reduced problem.

With the aid of B-splines [18], they proved some theoretical results and usedthese to derive the desired error estimates.

In another work, de Hoog and Weiss[30] have analyzed the application of collocation methods to singular problems such as one considered by the same authors in [29]. They showed that collocation gives the same results for singular boundary value problems as for non-singular problems.

Elder [38] showed how to apply the subscheme of invariant imbedding known as integration to blow up to compute the smallest eigenlength of a linear first order systems having a singularity of first kind. The purpose of this paper is to define an invariant imbedding for the singular TPBVP and then give the appropriate initial conditions at the origin for the Ricatti differential equation. They showed that the smallest eigenlength of the singular TPBVP is the right endpoint of the maximal interval of existence of the Ricatti initial-value problems. With this result it is reasonable to consider computing this smallest eigenlength by integrating the Ricatti equation to its singularity or to "blow up". This method is referred to as "integration-to-blow up" in the papers by Boland and Nelson [15] and Nelson and Elder [70]. This procedure has also used in [15,70] with great success in the computation of eigenlengths of nonsingular TPBVP.

Nelson, Sagong and Elder [71] have considered a linear homogeneous first-order differential system with a singularity of the first kind at $z = 0$,

$$u'(z) = (\frac{A_o}{z} + A_1(z))u(z) + (\frac{B_o}{z} + B_1(z))v(z),$$
$$(1.20)$$
$$v'(z) = (\frac{C_o}{z} + C_1(z))u(z) + (\frac{D_o}{z} + D_1(z))v(z).$$

where u and v are respectively in m-vector and an n-vector of dependent variables, and the matrices A_i, B_i, C_i, D_i for $i = 0,1$ are of the appropriate dimensions (e.g. A_i is mxm). The matrices A_o, B_o, C_o, and D_o are constant, and A_1, B_1, C_1, D_1 are analytic on $(0,\delta]$ for some $\delta > 0$ and piecewise continuous on $[0,\infty)$, with the boundary conditions of the form

$$u(0+) \text{ and } v(0+) \text{ exist (finite)}$$

and (1.21)

$$v(x) = \beta, \quad x > 0.$$

They showed how the approach of Elder can be adapted to the solution of (1.20) - (1.21) by means of Scott's version [85] of invariant imbedding.

Recently Chawla [21] discussed the construction of three point finite difference approximation and their convergence unaer appropriate conditions for the class of singular BVP's of the form

$$(x^{\alpha}y')' = f(x,y),$$
$$y(0) = A; \qquad 0 < \alpha < 1 \qquad (1.22)$$
$$y(1) = B,$$

The author established a certain integral identity on a general mesh from which the various methods are derived. For a non-uniform mesh over $[0,1]$, a method based on an evaluation of f* is obtained. For a uniform mesh, two methods based on three evaluations of f are obtained. When $\alpha = 0$, the method reduces to a classical second order method based on one evaluation of f. However $O(h^2)$ convergence for all the defined methods is established.

More recently Doedel [35, 36] have constructed some high order finite difference methods for non-singular two point boundary value problems. Doedel and Reddien [37] have extended these methods to an important class of singular boundary value problems considered by Jamet [50] and other authors. A compact finite difference approximation the the differential equation have been considered and these have been shown to be equivalent to the collocation scheme.

1.4 Boundary value problems on Infinite intervals :

Another type of singular problems is the study of solutions on unbounded interval, if the interval of interest is infinite or semi-infinite, where infinity is a regular singular point. For instance, the interval $0 \le x \le \infty$ sometimes called a semi-infinite interval, since it does have one finite end point, a boundary condition would normally be imposed at $x = 0$, due to no boundary exists on the other end. These problems arise in many branches of science and Engineering. Problems of practical importance frequently occur in Fluid dynamics,

Aerodynamics, Quantum Mechanics **etcetera.**

Often in most cases, the analytical solutions for these problems are not readily attainable and thus the problem is brought to the problem of finding efficient computational algorithms for obtaining numerical solution. Numerical methods for infinite or semi-infinite interval problems have been discussed by some authors. One of the ways of solving these problems is based on truncating the unbounded domain to a large but finite region. But one must make the decision as to how large the domain must be in order to properly represent an infinite or semi-infinite domain in the computational sense. A method for solving linear two-point boundary value problem on an infinite interval

$$L[y] \equiv y'' + p(x)y' + q(x)y = f(x)$$
$$y(a) = \alpha, \qquad y(\infty) = 0 \tag{1.23}$$

is given by Fox [42,43,44]. Applying the second boundary condition at a finite point $x = N$, N arbitrary, the solutions are computed by taking different values of N and observing the variations in the solutions till the desired accuracy is achieved.

Robertson [80] has discussed a second order finite difference scheme for solving the Infinite interval problem given by (1.23). The objective of his paper is to obtain numerical solution in a relatively small finite interval. The

method proposed is to examine $y^N(x)$, the solution of $Ly = f$ with $y(a) = \alpha$, $y(b^{(N)}) = 0$ under conditions which ensure $y^N(x) \to y(x)$ as $N \to \infty$. The results are shown to have $O(h^2)$ convergence. Several authors [49,67] adapted the procedure of choosing a large point to represent infinity before computing the numerical solutions.

In another work, Alspaugh [5] studied the application of Invariant imbedding to the solution of boundary value problem on infinite interval. By using invariant imbedding, the author converts the boundary value problem to initial value problems and the resulting Ricatti's equations are integrated numerically until the desired accuracy is obtained. For certain ill-conditioned problems, the usual methods of solution of two point boundary value problems fail. It has been shown that the numerical stability of invariant imbedding formulation permits the easy solution of such problems. Several criteria for determining the appropriate length of integration are presented.

Another way of solving the infinite interval problems is to reformulate the boundary value problem in a standard form. In such cases, one may use the coordinate transformations (Algebric or exponential transformation) to reduce the given problem to the problem over a finite interval. This procedure has been adopted earlier by several authors. Recently, Grosch and Orszag [46] investigated the utility of transformation techniques to solve boundary value problems in infinite regions. The utility of transformation has been shown through some

physical examples. However the great disadvantage of this approach is that the transformation technique usually produces a singular problem, which has an irregular singularity. Solutions that vanish rapidly or approach a constant at infinity are readily treated by mapping, but solutions that oscillate out to infinity are not so amenable to these techniques. The obvious advantage of these transformation is that no experimental choice of a large number, which represents the point at infinity is necessary.

In a recent survey, Ascher and Russell [8] have shown how various non-standard problems can be transformed to fit a simple format. Suppose a single equation expressing a boundary condition involves the value of the solution of the differential equation at more than one point; it is shown how the problem can be formulated so that each boundary condition involves only one of the boundary points. Suppose a problem involves a boundary condition at an unknown point, it is shown how to obtain an equivalent problem with known boundary points. Also reformulations to remove singularities and infinite intervals are discussed.

Recently boundary value problems over semi-infinite intervals have been studied by Lentini and Keller [61-62]. The authors deal with two point boundary value problems of the following forms

(a) $y'(t) = A(t)y(t) + f(t), \quad t_o \leq t < \infty$; with conditions

(b) $\sup_{t \geq t_o} ||y(t)|| < \infty$; (1.24)

(c) $B_o y(t_o) + \lim_{t\to\infty} B_\infty y(t) = \beta$ (β = a constant vector) ;

and

(a′) $\frac{du(t)}{dt} = f(t,u(t)), \quad t_o \leq t < \infty$; with conditions

(b′) $\lim_{t\to\infty} u(t) = u_\infty$ exists; (1.25)

(c′) $b_o(u(t_o),u_\infty) = 0,$

under suitable smoothness conditions for the matrix $A(t)$ and the vector $f(t,u(t))$ and for appropriate constant matrices B_o, B_∞ and vector b_o. The technique of the reduction to a finite interval problem is adopted and its correct implementation is shown. The basic idea employs that for linear problems the space S_B of bounded solutions is finite dimensional and is easily determined. Then the proper 'boundary condition at infinity' is simply that the projection of the solution P_n to the complement of S_B must vanish. Existence, uniqueness and behaviour of the solutions at infinity are discussed. The appropriate projection condition is simply applied to a finite point to obtain a finite domain. However a priori estimates for the location of finite boundary are not easy to obtain. In another work, the application of the technique has been shown by the same author for the Von Karman Swirling flows [61], and a linear elasticity problem [60].

Recently a complete treatment, which give the asymptotic behaviour of the solution has been presented by some authors. F.R. De Hoog and Weiss [32] solved an infinite interval problem by restricting the problem to a large but Finite interval and imposing certain supplementary conditions at the far end. The success of this procedure depends upon the proper choice of these conditions. For a rather general class of problems the authors give a characterization of all possible supplementary boundary condition that work and examine the rate of convergence of the finite problem to that of original problem as the interval length of the finite problem tends to infinity and describe the boundary condition for which this rate is optimal.

Markowich [64] formulated a adhoc method to solve boundary value problem on infinite interval of the form

$$y' = t^{\alpha} f(t,y), \qquad 1 \leq t < \infty, \quad \alpha \in \mathbb{N}_0 \tag{1.26}$$

$$y \in C([1,\infty]) \Longleftrightarrow y \in C\,[1,\infty)) \text{ and } \lim_{t\to\infty} y(t) \text{ exists}$$

where f : $b(y(1)) = 0$

where $f : R^{n+1} \to R^n$ and N_0 is the set of nonnegative integers. The author deals with the numerical solution of boundary value problem by truncating the infinite interval to a finite but large one and to impose additional boundary condition at the for end. These boundary conditions should be posed in a way so that they express the asymptotic behaviour of the actual solution.

The resulting boundary value problem can be reduced the following form :

$$x'_T = t^{\alpha} f(t, x_T), \qquad 1 \le t \le T,\ t \gg 1,$$

$$b(x_T(1)) = 0 \tag{1.27}$$

$$S(x_T(T), T) = 0$$

In another paper, Markowich [65] studied the solution of the system

$$y' = t^{\alpha} f(t, y), \qquad 1 \le t < \infty,\ \alpha \ge 0 \tag{1.28}$$

with separated boundary conditions at 1 and ∞ where appropriate asymptotic boundary conditions are determined at ∞ to ensure a smooth solution. Asymptotic analysis of solution behaviour is used to determine the point $T = T(\varepsilon)$ such that the solution to a regular BVP on $[1, T]$ is within $O(\varepsilon)$ of the original solution. Certain symmetric (spline) collocation schemes are analyzed for solving this BVP. By equidistributing truncation errors, meshes with exponentially increasing subinterval lengths, the solutions with $O(\varepsilon)$ accuracy are produced. The authors also show that the condition number of the collocation equations is asymptotically proportional to the number of mesh points employed when using this exponentially graded mesh. For K Gauss points collocation, this is only $O(\varepsilon^{-1/2K})$. Stability as $\varepsilon \to 0$ $(T(\varepsilon) \to \infty)$ is shown for the linear case.

1.5 Essential Singularities :

Recently the numerical solution of boundary value problems with an essential singularity has been investigated by Hoog and Weiss [31]. The boundary value problems of the type

$$t^{\alpha}y' = f(t,y), \quad 0 < t \leq 1, \quad y \in C[0,1] \cap C'(0,1]$$
$$b(y(0),y(1)) = 0 \tag{1.29}$$

where $\alpha \geq 1$, y is n vector, and f and b are nonlinear mappings on suitable domains. Problems on semi-infinite or infinite intervals on the other hand usually leads to the case $\alpha > 1$ (singularity of the second kind). The author's have introduced a canonical form for the system (1.28) which provides a basis for the analysis of such boundary value problems. They also established a Fredholm theory for linear problems in this canonical form and derived existence and regularity results for the solutions of nonlinear problems.

The numerical solution of (1.28) with $\alpha = 1$, assumed to be in canonical form, has been studied by Hoog and Weiss [29]. Here they extend the results to the general case $\alpha \geq 1$. The centered Euler scheme and the trapezoidal scheme is then used to solve the regular boundary value problem. By using Fredholm theory, the authors obtain the modified appropriate boundary condition for the difference method. They also show for important problems the error has an $O(h^2)$ expansion, which renders possible the use of Richardson extrapolation or related

technique. The applicability of the method has been illustrated by Blasius equation and a problem arising in the study of electro-magnetism.

This is the only paper dealing with essential singularities that the author has been able to find in the literature.

1.6 Summary of the thesis :

In the present thesis, some new and efficient numerical methods have been developed for solving singular boundary value problems over finite and infinite intervals. The thesis comprises of eight chapters.

In the second chapter, a particular class of singular boundary value problems have been considered for ordinary differential equations on a finite interval, which has a singularity of the first kind. These types of problems have been discussed earlier by Jamet [50] and arise when reducing partial differential equations by physical symmetry. The singularity is subtracted out by using the series expansion and a new boundary condition is derived in the vicinity of the singularity. A discrete invariant imbedding method has been developed to solve the resulting regular boundary value problem efficiently. The stability of the method is discussed. The proposed method is conceptually simple and easy to implement. Some test examples have been solved and the numerical results presented. A comparison of numerical results has also been made with other methods.

Chapter 3 deals with the continuous version of Invariant Imbedding method to solve the singular boundary value problems considered in Chapter 2. Again the expansion procedure has been employed to derive the new boundary condition near to singularity. Next a continuous invariant imbedding has been described to reduce the regular boundary value problem in to a set of initial value problems. Runge Kutta Fehlberg variable step size technique has been employed to integrate the stable initial value problems efficiently. Some model problems have been solved to illustrate the efficiency of the method. The continuous invariant imbedding combined with variable step size Initial value software have been found to be more accurate than the discrete version of invariant imbedding but at a slightly more cost of computational time.

The treatment given to the singularities to the problems considered in earlier chapters is based on using extended power series and thereby derive a new boundary condition near to singularity. However, in cases where there is slow convergence of the series expansion, an economized expansion may be used. In chapter 4, we discuss Chebyshev economization near the singular point to overcome slow convergence of the series. Using the shifted Chebyshev polynomials and the Lanczos Tau method, a new boundary condition near the singularity is obtained. The resulting regular boundary value problem is then treated with continuous Invariant Imbedding described in Chapter 3. Numerical results of some test examples are also included.

The attempts in earlier chapters for the removal of singularity are based on using expansion procedures in the neighbourhood of the singularity. However for some problems, it may be difficult or even not possible to obtain the series expansion near the singularity. In such cases, one may have to use a direct approach to solve singular boundary value problems. A modified fourth order finite difference method to solve a certain class of linear singular BVP's is presented in Chapter 5. The original differential equation is modified at the singular point. The main feature of the modified difference scheme is that it leads to the tridiagonal system of equations, which has been solved by discrete Invariant Imbedding method. Some model problems have been solved and the numerical results included.

The numerical solution of nonlinear singular boundary value problems has been discussed in Chapter 6. A quasilinearization technique has been used to reduce the nonlinear problem to a sequence of linear problems. A fourth order finite difference method described in Chapter 5 has been employed to solve these problems effectively. Some model problems have been solved to demonstrate the efficiency of the method.

In Chapter 7, we have considered the infinite interval boundary value problems in ordinary differential equations. In Case I, we derive the asymptotic boundary condition to represent the infinity condition at the far end. This boundary condition has been derived such that it expresses the asymptotic behaviour of the solution as well, and converge to the actual solution of

the 'infinite' problem as the length of finite interval tends to infinity. The resulting boundary value problem is treated by imbedding methods. The stability of the problem is analysed. In Case II, we have briefly included the transformation technique as an alternative method to solve these problems. For the transformed problems on a finite interval with a regular singularity at one end point of the interval, the method discussed in earlier chapters can be applied directly.

Finally in Chapter 8, the application of cubic spline method to infinite interval problems is discussed. By reducing the infinite interval to a finite interval which is large and imposing the asymptotic boundary conditions at the far end, the two point boundary value problem on a finite interval is treated by using cubic spline approximation. The tridiagonal system resulting from the spline approximation is efficiently solved by the method of imbedding. The stability of the method is also discussed and the theory is illustrated by test examples.

In a nut-shell, the numerical methods presented in this thesis for solving singular boundary value problems over finite and infinite intervals have been shown to be efficient over other methods. Although problems with singularity at one end point have been discussed, yet one may apply these methods to problems with interior regular singularities or two regular singular end points. The invariant imbedding methods is conceptually simple, easy to implement, and has the properties

of solving boundary value problems subject to different boundary conditions without extra computational effort.

Model problems have been solved and numerical results presented in respective chapters. The numerical results presented, in this thesis have been computed on DEC-1090 system in single precision arithmetic.

CHAPTER II

DISCRETE INVARIANT IMBEDDING FOR SINGULAR BOUNDARY VALUE PROBLEM

2.1 Introduction: As mentioned in Chapter 1, the numerical methods for approximating the solution of singular two point boundary value problems for ordinary differential equations are important in view of the frequent occurrence of these problems in Engineering and Science. Specific complete algorithms are classified according to, how the transformed problem is modeled discretely, and how the discrete model is solved efficiently. Due to the effect of singularity either in the differential equation or in the boundary condition, one may need extra care to solve these problems by efficient computational techniques.

We consider our analysis for the differential equation of the form

$$Ly \equiv y''(x)+p(x)y'(x)+q(x)y(x) = r(x) \qquad (2.1)$$

on the interval $x_o < x < b$, where $p(x)$ and $q(x)$ fail to be analytic at x_o. We demand $y(x)$ to be twice differentiable on $[x_o,b]$ and its second derivative to be continuous on $(x_o,b]$. We also assume that there exists a number σ, $0 < \sigma < 1$, such that $p(x) < \frac{\sigma}{x}$ for x small and $q(x) < 0$, then the two point boundary value problem

$$\begin{aligned} Ly(x) &= r(x), \qquad x_o < x \leqslant b \\ y(x_o) &= \alpha \\ y(b) &= \beta \end{aligned} \qquad (2.2)$$

$$y \in C^2(x_o,b] \cap C[x,b]$$

has a unique solution. For the one point boundary value problem

$$
\begin{aligned}
& Ly(x) = r(x), \qquad x_o < x < b \\
& y(b) = \beta \\
& y \in C^2(x_o,b] \cap [x_o,b]
\end{aligned}
\tag{2.3}
$$

with $\sigma \geq 1$ such that $p(x) > \frac{b}{x} - C$, where C is a nonnegative constant and $q(x) < 0$, the problem (2.3) has a unique solution. For one point boundary value problem we do not impose a value on $y(x)$ at $x = x_o$; the only requirement is that at the singular point $y(x)$ be bounded.

A particular class of this singular boundary value problem in ordinary differential equation arises as a result of the application of separation of variables to the equation of the generalized axially symmetric potential in a rectangle and has been studied by Parter [72], using finite difference scheme. Jamet [50] studied the problems (2.2)-(2.3) with the application of a standard three-point finite difference scheme with a uniform mesh size h and has shown certain convergence results. Those results appear as particular cases of general results for partial differential equations of elliptic-parabolic type which are given by Parter [72].

Gustaffsson [47] has given a numerical method for solving singular boundary value problems by representing the solution as series expansions in the vicinity of the singularity and by using difference methods for the remaining

interval. For linear systems of first order, Brabston and Keller [16] have used the same procedure in the neighbourhood of the singularity and used the Box scheme [57,58] for the solution of regular boundary value problems.

In this chapter we have presented a computational technique for the numerical solution of singular two point boundary value problems of the form (2.2). By employing the expansion technique on $(x_o,\delta]$, where $\delta > x_o$, near the singularity, we derive a new boundary condition at $x = \delta$. A discrete invariant imbedding is then described to solve the problem over the reduced interval. The stability analysis of the method is discussed. Numerical results for the model problems solved, have been presented and their comparisons made with other methods.

2.2 Removal of Singularity :

We shall first briefly describe how to replace the singular problem by a regular problem on an interval $[\delta,b]$, $\delta > x_o$. We consider a linear singular two point boundary value problem

$$Ly(x) \equiv y''(x)+p(x)y'(x)+q(x)y(x) = r(x) \; ; x_o < x \le b \qquad (2.4)$$

subject to boundary conditions

$$\begin{aligned} y(x_o) &= c \\ y(b) &= d \end{aligned} \qquad (2.5)$$

where x_o is a regular singularity. Under the assumptions

pointed out in Sec.2.1, for the Eqns (2.4)-(2.6) the solution exists and it is unique.

For the regular singular point $x = x_o$, we make use of the modified series expansion in a small interval near $x = x_o$, so that the Eqn. (2.4) has a solution of the form (see Coddington and Levinson [25])

$$y(x) = (x-x_o)^p \sum_{n=0}^{\infty} a_n (x-x_o)^n , \quad a_o \neq 0 \tag{2.7}$$

Differentiating (2.7) twice and using in (2.4), and comparing the coefficients of powers of $(x-x_o)$ on both sides, the values of p as the roots of the indicial equation and the recurrence relation for the coefficients a_n's are obtained. Depending upon the nature of the roots of the indicial equation, the general solution of Eqn. (2.4) can be written as

$$y(x) = \sum_{i=1}^{n} \alpha_i \, S_i(x) + S_{n+1}(x), \quad n \leq 2 \tag{2.8}$$

for $x \in (x_o, \delta]$, where $S_1(x)$ and $S_2(x)$ are two linearly independent solutions of the homogeneous equation corresponding to (2.4) and $S_{n+1}(x)$ is the particular solution of (2.4). The basic theortical results about these expansions about a **singular** point have been reviewed by Keller [55]. The series expansion may be valid for the entire interval $(x_o, b]$, however due to slow convergence of this series expansion, we restrict the expansion in the interval $(x_o, \delta]$, where $x_o < \delta \leq x \leq b$. We derive the regular boundary value problem

with a new boundary condition as follows. From Eqn. (2.8), at $x = \delta$,

$$\alpha_1 S_1(\delta) + \alpha_2 S_2(\delta) + S_{n+1}(\delta) = y(\delta) \tag{2.9}$$

and differentiating Eqn. (2.8), at $x = \delta$.

$$\alpha_1 S_1'(\delta) + \alpha_2 S_2'(\delta) + S_{n+1}'(\delta) = y'(\delta) \tag{2.10}$$

where the primes denote differentiation with respect to x.
We solve Eqns. (2.9)-(2.10) for α_1 and α_2 as

$$\alpha_1 = \frac{[y(\delta)-S_{n+1}(\delta)]S_2'(\delta)-[y'(\delta)-S_{n+1}'(\delta)]S_2(\delta)}{S_1(\delta)S_2'(\delta) - S_2(\delta)S_1'(\delta)} \tag{2.11}$$

$$\alpha_2 = \frac{[y'(\delta)-S_{n+1}'(\delta)]S_1(\delta)-[y(\delta)-S_{n+1}(\delta)]\, S_1'(\delta)}{S_1(\delta)S_2'(\delta) - S_2(\delta)S_1'(\delta)} \tag{2.12}$$

Also we have from Eqns. (2.5) and (2.8) at $x = x_o$,

$$\begin{aligned} \alpha_1 S_1(x_o)+\alpha_2 S_2(x_o)+S_{n+1}(x_o) &= y(x_o) \\ \alpha_1 S_1(x_o)+\alpha_2 S_2(x_o) &= y(x_o)-S_{n+1}(x_o) \end{aligned} \tag{2.13}$$

Using Eqns. (2.11), (2.12) and (2.13), we have

$$\frac{g(\delta)S_2'(\delta)-g'(\delta)S_2(\delta)}{h(\delta)} S_1(x_o)+ \frac{g'(\delta)S_1(\delta)-g(\delta)S_1'(\delta)}{h(\delta)} S_2(x_o)$$
$$= c-S_{n+1}(x_o) \tag{2.14}$$

where $g(x) = y(x)-S_{n+1}(x)$ and $h(x) = S_1(x)S_2'(x)-S_2(x)S_1'(x)$.
Eqn. (2.14) can be conveniently written as

$$[S_2'(\delta)S_1(x_o)-S_1'(\delta)S_2(x_o)]g(\delta) + [S_1(\delta)S_2(x_o)-S_2(\delta)S_1(x_o)]g'(\delta)$$
$$= h(\delta)[c-S_{n+1}(x_o)] \tag{2.15}$$

or

$$\alpha y(\delta)+\beta y'(\delta) = \gamma \tag{2.16}$$

where

$$\alpha = [S_2'(\delta)S_1(x_o)-S_1'(\delta)S_2(x_o)] \tag{2.17}$$

$$\beta = [S_1(\delta)S_2(x_o)-S_2(\delta)S_1(x_o)] \tag{2.18}$$

and

$$\gamma = h(\delta)[c-S_{n+1}(x_o)]+\alpha S_{n+1}(\delta)+ \beta S'_{n+1}(\delta) \tag{2.19}$$

Thus a regular boundary value problem over $[\delta,b]$ is given by Eqn. (2.4) with boundary conditions (2.16) and (2.6).

2.3 Discrete Invariant Imbedding :

The discrete invariant imbedding technique is motivated by the fact that it is very simple and easy to implement from the computational point of view. Several apparently different expositions on invariant imbedding have appeared in the literature. (See, for example, Casti and Kalaba [19], Meyer [66], Angel and Bellman [7]).

We describe the method of discrete invariant imbedding for the reduced regular boundary value problem given by Eqns.(2.4),(2.16) and (2.6). A unique solution of the problem given by (2.4),(2.16) and (2.6) exists if $p(x)$, $q(x)$, $r(x)$ are continuous on $[\delta,b]$ and $q(x)$ is negative there. Since these functions are continuous on a closed bounded interval, there must exist positive constants p^*, q^* and q_* such that

$$|p(x)| \le p^*,\ 0 < q_* \le q(x) \le q^*,\ \delta \le x \le b.$$

We now divide the interval $[\delta,b]$ into n equal parts as $\delta = x_o < x_1 < x_2 \ldots < x_n = b$ where $x_i - x_{i-1} = h$, $(i = 1,2,\ldots,n)$. Employing central difference approximations for the first and second order derivatives, the Eqn. (2.4) is discretized as

$$\frac{y_{i+1}-2y_i+y_{i-1}}{h^2} + p_i \frac{y_{i+1}-y_{i-1}}{2h} + q_i y_i = r_i \qquad i = 0,1,2,\ldots,n-1 \tag{2.20}$$

where p_i, q_i and r_i denote $p(x_i)$, $q(x_i)$ and $r(x_i)$ respectively. The difference Eqn. (2.20) can be written in a tridiagonal form as,

$$-A_i y_{i+1} + B_i y_i - C_i y_{i-1} = D_i \qquad i = 0,1,2,\ldots,n-1 \tag{2.21}$$

where

$$A_i = 1 + hp_i/2 \tag{2.22}$$

$$B_i = 2 - h^2 q_i \tag{2.23}$$

$$C_i = 1 - hp_i/2 \tag{2.24}$$

and

$$D_i = h^2 r_i \tag{2.25}$$

Consider now the coupled difference equations by writing Eqn. (2.21) as

$$v_{i+1} = y_i \tag{2.26}$$

$$y_{i+1} = M_i y_i - N_i v_i - O_i \tag{2.27}$$

where $M_i = B_i/A_i$; $N_i = C_i/A_i$ and $O_i = D_i/A_i$.

The boundary condition are discretized as

$$\alpha y_o + \beta \frac{(y_1 - y_{-1})}{2h} = \gamma \tag{2.27}$$

$$y_n = d \tag{2.28}$$

We seek a solution to Eqns. (2.25)-(2.26) in the form

$$v_i = W_i y_i + T_i \ , \qquad i = 0,1,2,..,n-1 \tag{2.29}$$

where W_i and T_i represents $W(x_i)$ and $T(x_i)$ respectively. By rewriting Eqn. (2.29) and using (2.25)-(2.26) to relate W_{i+1} and T_{i+1} with W_i and T_i we have,

$$\begin{aligned} y_i &= W_{i+1}(M_i y_i - N_i v_i - O_i) + T_{i+1} \\ &= W_{i+1}(M_i y_i - N_i(W_i y_i + T_i) - O_i) + T_{i+1} \\ &= (W_{i+1}(M_i y_i - W_{i+1} N_i W_i y_i) + (T_{i+1} - W_{i+1} O_i - W_{i+1} N_i T_i) \\ &= (W_{i+1} M_i - W_{i+1} N_i W_i) y_i + (T_{i+1} - W_{i+1} O_i - W_{i+1} N_i T_i) \end{aligned}$$

we match the coefficients in y_i to obtain the relations

$$W_{i+1} = \frac{1}{(M_i - N_i W_i)} \tag{2.30}$$

and

$$T_{i+1} = (W_{i+1} O_i + W_{i+1} T_i N_i) \tag{2.31}$$

The Eqn. (2.30)-(2.31) give the recursion relations for W_{i+1} and T_{i+1} for $i = 0,..,n-1$. To obtain W_{i+1} and T_{i+1} we need to know the value of W_i and T_i at $i = 0$. To do this we have from Eqn. (2.27) as,

$$y_1 = \frac{2h\gamma}{\beta} + y_{-1} - \frac{2h\alpha}{\beta} y_o \tag{2.32}$$

But from Eqn. (2.21) at $x = x_o (= \delta)$ we have

$$-A_o y_1 + B_o y_o - C_o y_{-1} = D_o \tag{2.33}$$

Now using (2.32) and (2.33) we get,

$$-A_o\left[\frac{2h\gamma}{\beta} + y_{-1} - \frac{2h\alpha}{\beta} y_o\right] + B_o y_o - C_o y_{-1} = D_o$$

$$y_o\left[\frac{2A_o h\alpha}{\beta} + B_o\right] - [A_o + C_o] y_{-1} = \left[D_o + \frac{2A_o h\gamma}{\beta}\right]$$

$$y_{-1}[A_o + C_o] = \left[B_o + \frac{2A_o h\alpha}{\beta}\right] y_o - \left[D_o + \frac{2A_o h\gamma}{\beta}\right]$$

$$y_{-1} = \frac{\left[B_o + \frac{2A_o h\alpha}{\beta}\right]}{[A_o + C_o]} y_o - \frac{\left[D_o + \frac{2A_o h\gamma}{\beta}\right]}{[A_o + C_o]} \tag{2.34}$$

Comparing the Eqns. (2.29) and (2.34), the initial values of W_o and T_o are obtained as,

$$W_o = \frac{\left[B_o + \frac{2A_o h\alpha}{\beta}\right]}{[A_o + C_o]} \tag{2.35}$$

and

$$T_o = \frac{-\left[D_o + \frac{2A_o h\gamma}{\beta}\right]}{[A_o + C_o]} \tag{2.36}$$

From the Eqns.(2.35)-(2.36) and (2.30),(2.31) we obtain the values of W_{i+1} and T_{i+1} in the forward process from $i = 0,1,2,\ldots,n-1$. To obtain the solution y_i , we have

$$y_{i+1} = M_i y_i - N_i v_i - O_i$$

$$= M_i y_i - N_i (W_i y_i + T_i) - O_i$$

$$= (M_i - N_i W_i) y_i - N_i T_i - O_i$$

$$y_i = \frac{(y_{i+1} + O_i + T_i N_i)}{(M_i - N_i W_i)} \qquad (2.37)$$

This equation can be used to find y_i where i ranges from n-1 to 0, in the backward process using the stored values of W_i and T_i and the boundary value $y_n = d$.

2.4 Computational Algorithm :

In order to compute the solution y_i's ($i = 0,..,n-1$), the computation is performed sequentially as follows :

Step 1 : Find the values of α, β and γ from Eqn. (2.19).

Step 2 : Calculate the values of W_0 and T_0 from Eqns. (2.35)-(2.36) and find the values of W_{i+1} and T_{i+1} ($i = 1,2,..,n-1$) in the forward process using the Eqns. (2.30)-(2.31)

Step 3 : Compute the value of y_i's ($i = n-1,..,0$) by using Eqn. (2.37) and the known W_i's and T_i's ($i = 0,...,n$) from Step 2 and using Eqn. (2.6).

2.5 Stability :

By stability we mean that the error made in one stage of the computations is not propagated into larger error

in succeeding calculations. Now we examine the stability for the recurrence relations given by Eqns. (2.30) and (2.31).

Let us assume E_i be a small error that has been introduced in the calculation of W_i , we then have

$$\tilde{W}_i = W_i+E_i \tag{2.38}$$

Thus instead of using Eqn. (2.30), we actually solve

$$\tilde{W}_{i+1} = \frac{1}{[M_i-N_i\tilde{W}_i]} \tag{2.39}$$

From Eqns. (2.38) and (2.39) we find the error at the next stage is given by

$$\begin{aligned} E_{i+1} &= (M_i-N_i\tilde{W}_i)^{-1} - (M_i-N_iW_i)^{-1} \\ &= [M_i-N_i(W_i+E_i)]^{-1}-(M_i-N_iW_i)^{-1} \\ &= (M_i-N_iW_i-N_iE_i)^{-1}-(M_i-N_iW_i)^{-1} \\ &= (M_i-N_iW_i-N_iE_i)^{-1}N_iE_i(M_i-N_iW_i)^{-1} \\ &\simeq (M_i-N_iW_i)^{-1} N_iE_i(M_i-N_iW_i)^{-1} \\ &= W_{i+1}^2 C_i/A_i E_i \end{aligned} \tag{2.40}$$

under the assumption that the error is initially small.

Assume that $N_i > 0$ for $0 \leq i \leq n-1$ and since $q(x) < 0$ it can be easily verified that $B_i \geq A_i+C_i$, for $0 \leq i \leq n-1$. From Eqn. (2.35) we have

$$W_o = (A_o+C_o)^{-1}[B_o + \frac{2A_oh\gamma}{\beta}]$$

and $|W_o| < 1$ if $M > 2$, where $M = h^2 q_o - \frac{h\gamma}{\beta} - \frac{h^2\gamma}{\beta} p_o$ (2.41)

under this condition and making use of the assumption on N_i, it follows very easily from (2.30) that

$$|W_i| < 1, \text{ for } i = 1,2,\ldots,n. \quad (2.42)$$

From Eqn. (2.40) it then follows that

$$|E_{i+1}| < |E_i| \text{ , provided } |C_i| < |A_i|$$

and thus making the recurrence relation stable.

Similarly for the other recurrence relation we have

$$\tilde{T}_i = T_i + \varepsilon_i \quad (2.43)$$

where ε_i is a small error, from Eqn. (2.31),

$$\tilde{T}_{i+1} = W_{i+1} O_i + W_{i+1} \tilde{T}_i N_i \quad (2.44)$$

We find the error in the next stage is given by

$$\begin{aligned} \varepsilon_{i+1} &= \tilde{T}_{i+1} - T_{i+1} \\ &= W_{i+1}\, \varepsilon_i N_i \end{aligned}$$

and so

$|\varepsilon_{i+1}| < |\varepsilon_i|$, $|W_i| < 1$, for $i = 1,2,..,n$ and the assumption $|C_i| < |A_i|$ making the relation (2.31) stable.

2.6 Numerical Results and Discussion :

In this section, the numerical results for the model problems are given. All computations were carried out in single precision arithmetic on DEC-1090 computer system.

Problem 2.1 : We consider the linear two point boundary value problem

$$y''(x) + \frac{\sigma}{x} y'(x) - \tau y(x) = 0, \qquad 0 < \sigma < 1, \quad \tau \geq 0$$

with boundary conditions

$$y(0) = 1$$
$$y(1) = 0$$

This is the model problem solved earlier by Jamet [50].

Problem 2.2 : Next we make the numerical experiments on the equation

$$y''(x) + \frac{\sigma}{x} y'(x) = -x^{1-\sigma} \cos x - (2-\sigma) x^{-6} \sin x, \qquad 0 < \sigma < 1$$

with boundary condition

$$y(0) = 0$$
$$y(1) = \cos 1.$$

This is the model problem considered by Gustaffsson [47], which has the exact solution $y(x) = x^{1-\sigma} \cos x$.

Problem 2.3 : Consider the linear two point boundary value problem

$$(x^{\alpha} y')' = \beta x^{\alpha+\beta-2} ((\alpha+\beta-1) + \beta x^{\beta}) y, \qquad 0 < x < 1,$$

with boundary conditions

$$y(0) = 1$$
$$y(1) = e.$$

This model problem has been taken from Chawla [21], which has the exact solution $y(x) = \exp(x^{\beta})$.

Problem 2.4 : We consider the problem

$$(x^{1/2}y')' - x^{1/2}y = -\frac{1}{2}(3+x^{-1/2})e^{-x}, \quad 0<x<1$$

subject to boundary conditions

$$y(0) = 1$$
$$y(1) = 2e^{-1}.$$

This is the model problem solved by Doedel and Reddien [37], which has the exact solution $y(x) = (x^{1/2}+1)e^{-x}$.

Problem 2.5 : As a last model problem, we have

$$y'' - \frac{0.5}{x}y' = -1 \qquad , \quad 0<x\leq 1$$

subject to boundary conditions

$$y(0) = 5$$
$$y(1) = 5$$

whose solution is $y(x) = 5-x^2+x^{3/2}$. This model problem has earlier been discussed by Ewa Weinmüller [92,93].

The numerical results for problem 2.1 at different mesh points for several mesh sizes and two different values of δ are presented in Tables 2.1 - 2.2 . It can be found that these results are much accurate than the results of Jamet [50]. To make it more apparent the comparison of our solutions for different mesh sizes is made with two other methods and presented in Table 2.5. It can be

observed that the numerical results obtained by the present method are quite comparable for any mesh size with the finite difference method of Jamet [50] and the collocation method of Reddien [73]. The solution at $x = 0.5$ for $\sigma = 0.5$ correct up to five significant places is known to be 0.25203 for this problem. Tables 2.3 - 2.4 present the solutions for the same example for a different value of σ and two choices of values of δ. For this value of σ, the comparison of the solution is made with the Jamet's solution [50] and presented in table 2.6.

In Table (2.7), the comparison of maximum errors in the solutions for problem 2.2 for different values of δ is made, and the errors in Gustaffsson's solutions correspond to the finite difference scheme of order two. The superiority of the solutions obtained by our method is again evident from the results.

In Table 2.8 the numerical results for the problem 2.3 are presented **for different values of h**. The results are given for $\beta = 4$ and $\alpha = 0.5$. To test the effect of singularity the values of δ are taken near to singularity. For problems 2.4 and 2.5, the results are shown in Tables 2.9 and 2.10. It can be observed from these tables that the computed solutions compare well with the exact solutions.

Table 2.1

Results for Problem 2.1

(σ = 0.5, τ = 1.0, δ = 0.5)

	h				
x	1/10	1/20	1/40	1/80	1/160
0.5	0.2509616	0.2517711	0.2519739	0.2520425	0.2520445
0.7	0.1363321	0.1367357	0.1368365	0.1368616	0.1368656
0.8	0.0873957	0.0876477	0.0877106	0.0877263	0.0877285
0.9	0.0422726	0.0423922	0.0424220	0.0424294	0.0424304

Table 2.2

Results for Problem 2.1

(σ = 0.5, τ = 1.0, δ = 0.2)

	h				
x	1/10	1/20	1/40	1/80	1/160
0.2	0.5019590	0.5065314	0.5076795	0.5079669	0.5080301
0.5	0.2495478	0.2514216	0.2518862	0.2520021	0.2520220
0.6	0.1892235	0.1906261	0.1909706	0.1910565	0.1910704
0.8	0.0869033	0.0875260	0.0876801	0.0877185	0.0877241
0.9	0.0420345	0.0423333	0.0424072	0.0424256	0.0424282

Table 2.3

Results for Problem 2.1

($\sigma = 0.2$, $\tau = 1.0$, $\delta = 0.5$)

x	h				
	1/10	1/20	1/40	1/80	1/160
0.5	0.3727644	0.3732550	0.3733774	0.3734079	0.3734118
0.7	0.2117490	0.2120046	0.2120681	0.2120838	0.2120841
0.8	0.1383073	0.1384698	0.1385101	0.1385201	0.1385198
0.9	0.0680450	0.0681234	0.0681428	0.0681476	0.0681473

Table 2.4

Results for problem 2.1

($\sigma = 0.2$, $\tau = 1.0$, $\delta = 0.2$)

x	h				
	1/10	1/20	1/40	1/80	1/160
0.2	0.6756758	0.6770162	0.6773548	0.6774390	0.6774540
0.4	0.4632033	0.4639039	0.4640781	0.4641208	0.4641227
0.5	0.3727149	0.3732428	0.3733736	0.3734055	0.3734049
0.6	0.2894291	0.2898205	0.2899173	0.2899407	0.2899389
0.8	0.1382890	0.1384653	0.1385087	0.1385192	0.1385174
0.9	0.0680360	0.0681212	0.0681422	0.0681472	0.0681462

Table 2.5

Comparison of Results for the problem 2.1
($\sigma = 0.5$, $\delta = 0.5$, $\tau = 1$)

$N = \frac{1}{h}$	Jamet's Method [50]	Reddien's Method [73]	Discrete Invariant imbedding
8	0.2903821	0.25305	0.2503571
16	0.2782581	0.25223	0.2516190
32	0.2700966	-	0.2519360
64	0.2645623	-	0.2520172
128	0.2607722	-	0.2520350
256	0.2581542	-	0.2520371

Table 2.6

Comparison of Results for the problem 2.1

($\sigma = 0.2$, $\delta = 0.5$, $\tau = 1.0$)

$N = \frac{1}{h}$	Discrete Invariant imbedding	Jamet's Method [50]
8	0.3723980	0.3830297
16	0.3731628	0.3789884
32	0.3733548	0.3766250
64	0.3734027	0.3752605
128	0.3734142	0.3744761
256	0.3734141	0.3740257

Table 2.7

Comparison of Maximum errors for the Problem 2.2 ($\sigma = 0.5$)

δ	Method	$N = \frac{1}{h}$			
		40	80	160	320
0.1	A	7.7×10^{-4}	1.7×10^{-4}	4.0×10^{-5}	9.6×10^{-6}
	B	1.1×10^{-3}	1.1×10^{-4}	1.2×10^{-5}	1.1×10^{-6}
0.2	A	1.6×10^{-4}	3.8×10^{-5}	9.1×10^{-6}	2.2×10^{-6}
	B	1.0×10^{-4}	1.1×10^{-5}	1.2×10^{-5}	1.4×10^{-6}
0.5	A	-	-	-	-
	B	1.5×10^{-5}	1.3×10^{-6}	1.3×10^{-6}	1.2×10^{-6}

A - Gustaffsson's Method

B - Discrete Invariant imbedding

Results for problem 2.3

$(\alpha = 0.5, \beta = 4.0)$

δ	x	h: 1/20	h: 1/40	h: 1/80	h: 1/160	Exact Solution
0.1	0.1	1.0032007	1.0008712	1.0002916	1.0001395	1.0001395
	0.2	1.0058306	1.0026590	1.0018644	1.0016557	1.0016013
	0.3	1.0131610	1.0093932	1.0084463	1.0081982	1.0081329
	0.5	1.0706713	1.0660469	1.0648804	1.0645794	1.0644944
	0.6	1.1450001	1.1400409	1.1387880	1.1384671	1.1384671
	0.7	1.2783340	1.2731294	1.2718133	1.2714780	1.2713764
	0.8	1.5131249	1.5079589	1.5066505	1.5063188	1.5062154
	0.9	1.9328586	1.9286767	1.9276152	1.9273475	1.9272618
0.2	0.2	1.0059822	1.0026996	1.0018749	1.00166070	1.0016013
	0.3	1.0132765	1.0094240	1.0084544	1.0082029	1.0081329
	0.5	1.0707340	1.0660636	1.0648849	1.0645833	1.0644944
	0.7	1.2783621	1.2731370	1.2718153	1.2714797	1.2713764
	0.8	1.5131412	1.5079633	1.5066518	1.5063193	1.5062154
	0.9	1.9328658	1.9286787	1.9276157	1.9273472	1.9272618
0.5	0.5	1.0720539	1.0663756	1.0649685	1.0646100	1.0644944
	0.6	1.1459598	1.1402827	1.1388492	1.1384890	1.1383730
	0.7	1.2789555	1.2732862	1.2718532	1.2714924	1.2713764
	0.8	1.5134848	1.5080497	1.5066738	1.5063274	1.5062154
	0.9	1.9330182	1.9287170	1.9276256	1.9273510	1.9272618

Table 2.9

Results for problem 2.4

δ	x	h: 1/20	h: 1/40	h: 1/80	h: 1/160	Exact Solution
0.1	0.1	1.195952	1.192214	1.191280	1.191020	1.190972
	0.2	1.188206	1.185700	1.185080	1.184889	1.184878
	0.3	1.149086	1.147198	1.146731	1.146573	1.146581
	0.5	1.036893	1.035775	1.035500	1.035389	1.035413
	0.6	0.975025	0.974190	0.973983	0.973896	0.973919
	0.7	0.912841	0.912249	0.912103	0.912037	0.912058
	0.8	0.851719	0.851342	0.851250	0.851204	0.851221
	0.9	0.792514	0.792334	0.792289	0.792267	0.792275
0.2	0.2	1.186474	1.185275	1.184974	1.184867	1.184878
	0.3	1.147705	1.146858	1.146647	1.146556	1.146581
	0.4	1.095100	1.094472	1.094314	1.094236	1.094268
	0.5	1.036033	1.035564	1.035446	1.035380	1.035413
	0.7	0.912375	0.912135	0.912074	0.9120314	0.912058
	0.8	0.851419	0.851269	0.851231	0.851201	0.851221
	0.9	0.792370	0.792298	0.792280	0.792264	0.792275
0.5	0.5	1.035657	1.035472	1.035424	1.035396	1.035413
	0.6	0.974088	0.973960	0.973926	0.973901	0.973919
	0.7	0.912170	0.912084	0.912062	0.912041	0.912058
	0.8	0.851288	0.851236	0.851223	0.851201	0.851221
	0.9	0.792306	0.792282	0.792276	0.792267	0.792275

Table 2.10

Results for problem 2.5

δ	x	h: 1/20	1/40	1/80	1/160	Exact solution
	0.1	5.021526	5.021598	5.021617	5.021615	5.021623
	0.2	5.049503	5.049459	5.049447	5.049422	5.049443
	0.3	5.074432	5.074348	5.074323	5.074276	5.074317
0.1	0.5	5.103687	5.103590	5.103554	5.103493	5.103557
	0.6	5.104878	5.104790	5.104755	5.104700	5.104758
	0.7	5.095761	5.095688	5.095657	5.095610	5.095662
	0.8	5.075613	5.075561	5.075536	5.075000	5.075542
	0.9	5.043853	5.043825	5.043811	5.043790	5.043815
	0.2	5.049366	5.049424	5.049436	5.049421	5.049447
	0.3	5.074306	5.074315	5.074311	5.074277	5.074317
	0.4	5.093003	5.092989	5.092976	5.092928	5.092982
0.2	0.5	5.103589	5.103565	5.103544	5.103496	5.103557
	0.7	5.095699	5.095673	5.095650	5.095614	5.095662
	0.8	5.075570	5.075550	5.075530	5.075503	5.075542
	0.9	5.043831	5.043820	5.043808	5.043792	5.043815
	0.5	5.103501	5.103542	5.103542	5.103540	5.103557
	0.6	5.104725	5.104751	5.104746	5.104742	5.104758
0.5	0.7	5.095642	5.095658	5.095650	5.095644	5.095662
	0.8	5.075531	5.075540	5.075531	5.075524	5.075542
	0.9	5.043811	5.043814	5.043808	5.043802	5.043815

CHAPTER III

CONTINUOUS INVARIANT IMBEDDING FOR SINGULAR BOUNDARY VALUE PROBLEMS

3.1 Introduction: The use of invariant imbedding techniques, in general, reduces the linear two point boundary value problems into a set of initial value problems. In the earlier chapter, a convenient discretized version of invariant imbedding has been developed for solving singular boundary value problem after its reduction to a regular problem by deriving a new boundary condition in the neighbourhood of the singular point. Though a reasonably good accuracy is obtained for a moderate step size h, yet one needs to take, as expected, a very fine mesh to achieve high precision in the solution especially when the point $x = \delta$ is very near to the singularity. This is due to the fact that the difference scheme of $O(h^2)$ would not, in general, give solutions correct upto second order near the singular point. The choice of a small step size is undesirable due to the fact that it leads to computational complexity.

To overcome these difficulties, we present another computational method on the basis of expansion technique and continuous version of invariant imbedding for solving singular boundary value problem considered in Chapter 2. The application of continuous version of invariant imbedding has been discussed in the literature by many authors. (see, for example, Bellman and

Kalaba [12], Chandrasekar [20], Bellman and Wing [13], Nelson and Scott [69], Kalaba and Kagiwada [53] and Denman and Mingle [34].

Sufficient conditions for existence of two versions of invariant imbedding for linear second order equations with a regular singular point have been considered by Scott [85]. The work of Scott constitutes a significant extension of earlier results of Banks and Kurowski [10]. Elder [38] showed how to apply the subscheme of invariant imbedding known as integration-to-blowup to compute the smallest eigenlength of linear first order system having a singularity of first kind. Nelson, Sagong and Elder [71] adapted Elder's approach to the solution of certain singular two point boundary value problems by means of Scott's version of invariant imbedding. Specifically, this approach applies to problems based on a linear homogeneous first order differential system with a singularity of first kind and with boundary conditions consisting of existence (finite) at the singularity and specified values at some second point.

In this chapter we have presented a numerical method for solving singular boundary value problem with a regular singular point at one end of the interval. The method is based upon the series expansion technique and continuous invariant imbedding. A new boundary condition at $x = \delta$ is derived by using series solution in the vicinity of singular point to substract out the singularity. The regular boundary value problem is then solved by employing a continuous invariant imbedding

method. Some numerical experiments have been included to demonstrate the applicability of the method.

3.2 Reduction to Regular Problem :

We shall consider a second order linear singular boundary value problem of first kind given by

$$y''(x) + F_1(x)y'(x)+F_2(x)y(x) = F_3(x), \quad x_o < x \le b \quad (3.1)$$

subject to boundary conditions

$$y(x_o) = \alpha \quad (3.2)$$

$$y(b) = \beta \quad (3.3)$$

where α and β are given constants.

Since $x = x_o$ is a regular singular point, we make use of the modified series expansion in a small interval $(x_o,\delta]$ so that the Eqn. (3.1) has a solution of the form

$$y(x) = (x-x_o)^p \sum_{n=0}^{\infty} a_n(x-x_o)^n, \qquad a_o \neq 0 \quad (3.4)$$

Differentiating (3.4) and substituting in (3.1) and comparing the coefficients of powers of $(x-x_o)$ on both sides, the values of p as the roots of the indicial equation and the recurrence relations for the coefficients a_k's are obtained. Depending upon the nature of the roots of the indicial equation, the general solution of (3.1) can be written as

$$y(x) = \sum_{i=1}^{m} \alpha_i R_i(x) + R_{m+1}(x), \qquad m \leq 2 \tag{3.5}$$

for $x \in (x_o, \delta]$, where $R_1(x)$ and $R_2(x)$ are two linearly independent solutions of homogeneous equation for (3.1) and $R_{m+1}(x)$ is the particular solution to (3.1). By taking the series expansion on $(x_o, \delta]$, the new boundary condition at δ is derived. We have from Eqn. (3.5),

$$\alpha_1 R_1(\delta) + \alpha_2 R_2(\delta) + R_{m+1}(\delta) = y(\delta) \tag{3.6}$$

$$\alpha_1 R_1'(\delta) + \alpha_2 R_2'(\delta) + R_{m+1}'(\delta) = y'(\delta) \tag{3.7}$$

where primes denote the differentiation. Equations (3.6) - (3.7) are solved for α_1 and α_2 as

$$\alpha_1 = \frac{[y(\delta)-R_{m+1}(\delta)]\, R_2'(\delta)-[y'(\delta)-R_{m+1}'(\delta)]\, R_2(\delta)}{R_1(\delta)R_2'(\delta) - R_2(\delta)R_1'(\delta)} \tag{3.8}$$

and

$$\alpha_2 = \frac{[y'(\delta)-R_{m+1}'(\delta)]\, R_1(\delta)-[y(\delta)-R_{m+1}(\delta)]\, R_1'(\delta)}{R_1(\delta)\, R_2'(\delta) - R_2(\delta)\, R_1'(\delta)} \tag{3.9}$$

Also from Eqns. (3.3) and (3.5), we have

$$\alpha_1 R_1(x_o) + \alpha_2 R_2(x_o) + R_{m+1}(x_o) = y(x_o) \tag{3.10}$$

Using the equations (3.8), (3.9) and (3.10) and using $y(x_o) = \alpha$, and after simple algebra, we have

$$A\, y(\delta) + B\, y'(\delta) = C \tag{3.11}$$

where

$$\begin{aligned} A &= [R_2'(\delta)\, R_1(x_o) - R_1'(\delta)\, R_2(x_o)] \\ B &= [R_1(\delta)\, R_2(x_o) - R_2(\delta)\, R_1(x_o)] \\ C &= h(\delta)\,[\alpha - R_{m+1}(x_o)] + A\, R_{m+1}(\delta) + B\, R'_{m+1}(\delta) \end{aligned} \tag{3.12}$$

with

$$h(\delta) = [R_1(\delta)\, R_2'(\delta) - R_2(\delta)\, R_1'(\delta)]$$

The Eqns. (3.1), (3.11) and (3.3) form a reduced regular boundary value problem over the interval $[\delta, b]$.

3.3 Continuous Invariant Imbedding :

In this section, we discuss the method of continuous invariant imbedding for solving the reduced problem over $[\delta, b]$. We follow on the lines of Scott's version of Imbedding [85,87] to reduce the boundary value problem into a sequence of initial value problems.

To be specific, we write Eqn. (3.1) as a systems of two first order equation in the form $y(x) = u(x)$; $\frac{d}{dx}(y(x)) = \frac{d}{dx}(u(x)) = v(x)$ and $\frac{dv(x)}{dx} = -F_1(x)v(x) - F_2(x)u(x) + F_3(x)$. Hence we may write Eqn. (3.1) in the form

$$\frac{du(x)}{dx} = v(x) \tag{3.13}$$

$$-\frac{dv(x)}{dx} = F_1(x)v(x) + F_2(x)u(x) - F_3(x) \tag{3.14}$$

where the minus sign on the left hand side of the Eqn. (3.14) is purely historical. The corresponding boundary conditions are

given by

$$A\,u(\delta) + B\,v(\delta) = C \tag{3.15}$$

$$u(b) = \beta \tag{3.16}$$

We now discuss the invariant imbedding for a more general first order system of the form

$$u'(x) = a(x)u(x)+b(x)v(x)+S^{+}(x) \tag{3.17}$$

$$-v'(x) = c(x)u(x) + d(x)v(x) + S^{-}(x) \tag{3.18}$$

where primes denote differentiation, with all functions $a(x)$, $b(x)$, $c(x)$, $d(x)$, $S^{+}(x)$ and $S^{-}(x)$ to be continuous and subject to boundary conditions given by (3.15) - (3.16). From the method of continuous invariant imbedding, we have the relations (see Scott [85]).

$$u(x) = S_1(x)\;v(x) + S_2(x)\;u(\delta) + S_3(x) \tag{3.19}$$

$$x \in [\delta, b]$$

$$v(\delta) = Q_1(x)\;v(x) + Q_2(x)\;u(\delta) + Q_3(x) \tag{3.20}$$

where the Eqn. (3.19) is the generalized Ricatti transformation and Eqn. (3.20) is the recovery transformation. The first term on the right hand side of Eqn.(3.1) represents the contributions from the homogeneous equation, the second term represents the contributions from the boundary conditions at $x = \delta$ and the last term represents contributions from the nonhomogeneous term in the equations. The transformations can be motivated from both a physical and mathematical point of view.

We shall now derive differential equations for the functions $S_1(x)$, $S_2(x)$, $S_3(x)$, $Q_1(x)$, $Q_2(x)$ and $Q_3(x)$. Differentiating (3.19) we have

$$u'(x) = S_1'(x)v(x)+S_1(x)v'(x)+S_2'(x)u(\delta)+S_3'(x) \qquad (3.21)$$

using Eqns. (3.17) and (3.18) in (3.21) we obtain,

$$a(x)u(x)+b(x)v(x)+S^+(x) = S_1'(x)v(x)+S_1(x)\{-c(x)u(x)$$
$$-d(x)v(x)-S^-(x)\} + S_2'(x)u(\delta)+S_3'(x)$$

or

$$a(x)\{S_1(x)v(x)+S_2(x)u(\delta)+S_3(x)\} + b(x)v(x)+S^+(x)$$

$$= S_1'(x)v(x)+S_1(x)\left[-c(x)\{S_1(x)v(x)+S_2(x)u(\delta)+S_3(x)\}\right.$$

$$\left.-d(x)v(x)-S^-(x)\right] + S_2'(x)u(\delta) + S_3'(x). \qquad (3.22)$$

or

$$v(x)\ \{S_1(x)a(x)+b(x)-S_1'(x)+c(x)S_1^2(x)+d(x)S_1(x)\}$$

$$+ u(\delta)\ \{S_2(x)a(x)+c(x)S_1(x)S_2(x)-S_2'(x)\} \qquad (3.23)$$

$$+\{S_3(x)a(x)+S^+(x)+S_1(x)S_3(x)c(x)+S^-(x)S_1(x)-S_3'(x)\} = 0$$

Eqn. (3.23) will be satisfied if each term in the braces to set equal to zero. That is

$$S_1'(x) = b(x) + [a(x)+d(x)]\ S_1(x)+c(x)S_1^2(x) \qquad (3.24)$$

$$S_2'(x) = [a(x) + c(x)\ S_1(x)]\ S_2(x) \tag{3.25}$$

$$S_3'(x) = [a(x)+c(x)S_1(x)]\ S_3(x)+S^-(x)S_1(x)+S^+(x) \tag{3.26}$$

suitable initial conditions suggested by (3.15) and (3.16) are

$$S_1(\delta) = 0\ ;\quad S_2(\delta) = 1\ ;\quad S_3(\delta) = 0. \tag{3.27}$$

Similarly differentiating (3.20) and using Eqns. (3.17) – (3.18), we obtain another set of equations,

$$Q_1'(x) = [d(x) + c(x)\ S_1(x)]\ Q_1(x) \tag{3.28}$$

$$Q_2'(x) = [c(x)\ Q_1(x)\ S_2(x)]\ Q_2(x) \tag{3.29}$$

$$Q_3'(x) = [c(x)\ S_3(x) + S^-(x)]Q_1(x) \tag{3.30}$$

with suitable initial conditions

$$Q_1(\delta) = 1\ ;\quad Q_2(\delta) = 0\ ;\quad Q_3(\delta) = 0 \tag{3.31}$$

One can easily verify that the above process does indeed solve the original linear problem. Thus sequence of initial value problems (3.24) – (3.31) are solved numerically by efficient initial value routines. Once $S_1(x)$, $S_2(x)$, $S_3(x)$, $Q_1(x)$, $Q_2(x)$ and $Q_3(x)$, $x \in [\delta, b]$ are known, the Eqns. (3.19) – (3.20) can be evaluated at $x = b$ to yield

$$u(b) = S_1(b)\ v(b) + S_2(b)\ u(\delta) + S^+(b) \tag{3.32}$$

$$v(\delta) = Q_1(b)\ v(b) + Q_2(b)\ u(\delta) + S^-(b) \tag{3.33}$$

Since $u(b)$ is known from Eqn. (3.16), we solve Eqns. (3.32), (3.33) and (3.15) as a system of linear equation for the unknowns $u(\delta)$, $v(\delta)$ and $v(b)$. Then Eqns. (3.19) and (3.20) are solved for $u(x)$ and $v(x)$ for all values of $x \in [\delta, b]$, by using the known values of $u(\delta)$, $v(\delta)$ and $v(b)$ respectively.

3.4 Computational Algorithm :

In order to compute the solution u, the computation is performed sequentially as under :

Step 1 : Integrate the initial value problems given by Eqns. (3.24) - (3.31), using efficient initial-value routines, from $x = \delta$ to $x = b$ to obtain the S_i and Q_i profiles and store them.

Step 2 : Find the values of A, B and C from Eqn. (3.15).

Step 3 : Evaluate the Eqns. (3.19) - (3.20) at $x = b$ using the values $S_i(b)$ and $Q_i(b)$, $(i = 1,2,3)$ from Step 1, and using $u(b)$ from the boundary conditions. The resulting equations would contain the unknowns $u(\delta)$, $v(\delta)$ and $v(b)$.

Step 4 : Combine the equations resulting from Step 3 with equation (3.15) and solve these three equations for the unknowns $u(\delta)$, $v(\delta)$ and $v(b)$.

Step 5 : Compute $v(x)$ and $u(x)$ for any $x \in [\delta, b]$ using the values of $u(\delta)$ and $v(\delta)$ from Step 4, and the stored values of S_i and Q_i from Step 1.

It may be noted that the Step 1, which incidently involves maximum computer time in the entire computational procedure, need not to be repeated if one has to solve different boundary value problems given by the same differential Eqn.(3.1) but different boundary conditions (3.2) - (3.3) but only Steps (2) - (6) be repeated for each set of boundary conditions, using the stored values of S_i and Q_i from Step 1 in each case.

3.5 Numerical Results and Discussion :

In this section we shall illustrate the use of the algorithm derived in the previous section by applying it to several examples. In our examples all the corresponding initial value problems (3.24) - (3.21) were solved by using a fourth-fifth order Runge Kutta Fehlberg scheme designed to estimate the local error and control step size for the accuracy requirements [40,41]. All computations were carried out in single precision on DEC-1090 computer system with a relative and absolute error of 10^{-5} and 10^{-13} respectively.

Problem 3.1 : We consider the linear two point boundary value problem

$$u''(x) + \frac{\sigma}{x} u'(x) - \tau u(x) = 0, \quad 0 < \sigma < 1, \quad \tau > 0$$

with boundary conditions

$$u(0) = 1$$

$$u(1) = 0$$

This problem has been studied earlier by Jamet [50].

Problem 3.2 : We solve

$$2x(1+x)\, y''' + (1+5x)\, y'' + y = 0$$

with boundary conditions

$$y(0) = 1$$

$$y(1.5) = 1$$

This problem has earlier been solved by Cohen and Jones [26] and has the exact solution given by $y(x) = \frac{(1 + \sqrt{x})}{(1 + x)}$.

Problem 3.3 : Next we make numerical experiments on the non-homogeneous equation

$$u''(x) + \frac{\sigma}{x} u'(x) = -x^{1-\sigma} \cos x - (2-\sigma) x^{-\sigma} \sin x, \quad 0 < \sigma < 1$$

with boundary condition

$$u(0) = 0$$

$$u(1) = \cos 1.$$

This example has been taken from Gustaffsson[47] and has the exact solution $u(x) = x^{1-\sigma} \cos x$.

The computed solution for Problem 3.1 for different values of δ when $\sigma = 0.5$ have been presented in Table 3.1. At the various values of x, the solutions compare very well with the analytical solution (series solution). The problem (3.1) has been earlier solved by Jamet [50] and Reddien [73] and their

computed solution at $x = 0.5$ for different mesh sizes have been given in Table 3.2. This table also contain solutions computed at $x = 0.5$ by Invariant imbedding using a Runge-Kutta-Fehlberg scheme with step size control to solve our initial value problems. Thus the step sizes h given in the Table 3.2 have no direct relevance to invariant imbedding solution. As in evident from this table, the invariant imbedding solution is much superior to the solution obtained by Jamet or Reddien for a very fine mesh. The behaviour of the solution when δ is very near to the singularity has been shown in Tables (3.3) – (3.4). It has been observed here that a comparatively smaller step size is required (as expected) to achieve the desired accuracy in the solutions.

The numerical solutions for problem 3.2 obtained by our method and the comparison of those solutions with Cohen's solutions have been given in Table (3.5). The solutions obtained by our method compare well with exact solution and that of Cohen's solutions.

Tables (3.6) – (3.7) give the numerical results for the problem 3.3. The computed solution at different points with respect to several values of δ are presented in Table 3.6. The comparison of maximum error incurred in the solutions obtained by our method and that of Gustaffsson has been made in Table (3.6). The superiority of our method in most of the cases is evident from the results.

TABLE 3.1

Results for the Problem 3.1

X	$\delta = 0.2$	$\delta = 0.4$	$\delta = 0.5$
0.2	0.5080600	–	–
0.4	0.3221206	0.3221289	–
0.5	0.2520316	0.2520420	0.2520425
0.9	0.0424309	0.0424321	0.0424322

TABLE 3.2

Comparison of Numerical Results for Problem 3.1

$(\sigma = 0.5,\ \tau = 1,\ x = 0.5)$

$N = \frac{1}{h}$	Jamet's Method [50]	Reddien's Method [73]	Invariant imbedding Method*
8	0.29038211	0.25305	0.25204250
16	0.27825809	0.25223	–
32	0.27009658	–	–
128	0.26077219	–	–
512	0.25633371	–	–

*The step size h has no direct relevance to Invariant imbedding solution and refers only to Jamet's and Reddien's solution.

TABLE 3.3

Results for the Problem 3.1

($\delta = 0.05$, $\sigma = 0.5$, $\tau = 1$)

X	u(X)
0.05	0.75006408
0.10	0.64846210
0.15	0.57142780
0.20	0.50806241
0.50	0.25204202
0.80	0.08773196
0.90	0.04243212

TABLE 3.4

Results for the Problem 3.1

($\delta = 0.125$, $\sigma = 0.5$, $\tau = 1$)

X	u(X)
0.125	0.60761680
0.250	0.45343930
0.375	0.34147399
0.500	0.25204244
0.625	0.17697532
0.750	0.11175222
0.875	0.53454321

TABLE 3.5

Results for the Problem 3.2 (δ = 0.5)

X	Imvariant Imbedding Solution	Cohen's Solution	Exact Solution
0.5	1.243902	1.243964	1.244017
0.6	1.217836	1.217871	1.217921
0.7	1.190924	1.190939	1.190997
0.8	1.640782	1.164078	1.164136
0.9	1.137794	1.137781	1.137840
1.0	1.112338	1.112319	1.112372
1.1	1.087842	1.087824	1.087868
1.2	1.064364	1.064348	1.064382
1.3	1.041912	1.041900	1.041924
1.4	1.020469	1.020462	1.020474

TABLE 3.6

Results for the Problem 3.3 (σ = 0.5)

X	δ = 0.1	δ = 0.2	δ = 0.4
0.1	0.31464841	–	–
0.2	0.43829967	0.43829892	–
0.3	0.52326032	0.52325916	–
0.4	0.58253142	0.58252991	0.5825301
0.6	0.63930355	0.63930194	0.6393022
0.8	0.62315431	0.62315313	0.6231534
0.9	0.58971162	0.58971087	0.5897109

TABLE 3.7

Comparison of Maximum Errors*

$N = \frac{1}{h}$	δ	Gustaffsson Solution	Invariant Imbedding Solution
40		1.5×10^{-5}	
80	0.1	7.2×10^{-7}	4.4×10^{-8}
160		4.0×10^{-8}	
40		7.9×10^{-7}	
80	0.2	4.4×10^{-8}	1.8×10^{-8}
160		2.6×10^{-9}	
40		3.7×10^{-8}	
80	0.4	2.1×10^{-9}	7.4×10^{-9}
160		1.3×10^{-10}	

*The step size h refers only to the Gustaffsson case.

CHAPTER IV

Singular boundary value problems Via Chebyshev Polynomials and Invariant imbedding

4.1 Introduction: The object of this chapter is to describe a method based on Chebyshev polynomials and Invariant imbedding to singular boundary value problems given in Chapter 2. We have observed that for a particular class of problems the series expansions may be suitable due to the nature of the physical situation of the defined problem, but in general it alone may not produce an effective approximation near the singularity. It is due to the fact that the series may converge slowly in the vicinity of the singularity thereby necessitating to include a large number of terms of the expansion to obtain a reasonably good accuracy. However an attempt is made here to reduce the necessary number of terms in the series expansion and without increasing the errors by the process called Chebyshev economization. This method effectively produces a good approximation and is based on the fundamental property of the Chebyshev polynomials.

Recently Cohen and Jones [26] studied a shifted Chebyshev polynomial with finite difference correction approach for a second order linear ordinary differential equation with a regular singular point. They considered these polynomials on the whole interval where the polynomials are valid, by neglecting the effect of singularity.

In this chapter we study the economized expansion procedure based on Chebyshev polynomials to remove the singularity for a singular two point boundary value problem. The new boundary condition is derived in the vicinity of the singularity. The invariant imbedding method discussed in Chapter 3 is used for numerically solving the reduced boundary value problem. Model problems have been solved and the numerical results are presented.

4.2 Economized Series Expansion :

For the sake of brevity, we consider a homogeneous linear ordinary differential equation given by

$$Ly \equiv y''(x)+F_1(x)y'(x)+F_2(x)y(x) = 0, \quad 0 < x \leq 1, \qquad (4.1)$$

with boundary conditions

$$y(0) = \alpha \qquad (4.2)$$

$$y(1) = \beta \qquad (4.3)$$

where $x = 0$ is the regular singular point of the differential equation (4.1). However if the interval under consideration is $[a,b]$, we transform it to the interval $[-1,1]$ by the change of variable,

$$x = \frac{1}{2}(b-a)\,t + \frac{1}{2}(b+a) \qquad (4.4)$$

and for the special range $0 \leq x \leq 1$, we can write

$$t = 2x - 1 \qquad (4.5)$$

Due to the singularity at $x = 0$, the solution of Eqn.(4.1) can be written as

$$y(x) = x^r \sum_{n=0}^{\infty} C_n x^n, \qquad C_o \neq 0 \tag{4.6}$$

The coefficients C_n's and the indicial roots r's can be obtained by differentiating (4.6) and substituting in (4.1), comparing the coefficients of powers of x on both sides of the equation. One may write the general solution as

$$y(x) = \sum_{i=1}^{2} \alpha_i \, R_i(x) \tag{4.7}$$

where $R_1(x)$ and $R_2(x)$ are two linearly independent solutions and α_1 and α_2 are arbitrary constants. In a situation where we have slow convergence of the series solution, we express the solution of (4.1) by a Chebyshev Economized expansion in $(0,\varepsilon]$, where ε is chosen near to singularity. It may be noted here that if the series solution corresponding to different indicial roots are different, one can remove the term x^m for negative and fractional m by the substitution $y = x^m u$ in (4.1) and carry out a similar analysis for the differential equation in u. It may also be noted here that we need to transform the Chebyshev polynomial $T_n^*(x)$ valid for $[0,1]$ to shifted Chebyshev polynomial $T_n^*(\bar{x})$ which are valid on $(0,\varepsilon]$, $\varepsilon \leq 1$ by the change of variable

$$\bar{x} = \frac{\varepsilon}{2}(x+1)$$

Let us assume that for different indicial values the series $R_1(x)$ and $R_2(x)$ are equal to $R(x)$ so that the general solution is of the form

$$y(x) = (\alpha_1 x^{m_1} + \alpha_2 x^{m_2}) R(x) \qquad (4.8)$$

where m_1 and m_2 are the roots of the indicial equation.

In order to approximate $R(x)$ by an economized expansion $p_N(x)$, we assume that $p_N(x) = \sum_{r=0}^{N} b_r x^r$ satisfies the differential equation

$$y''(x)+F_1(x)y'(x)+F_2(x)y(x) = \tau T_N^*(x/\varepsilon) \qquad (4.9)$$

where $T_N^*(x/\varepsilon)$ are the shifted Chebyshev polynomials in the interval $0 < x \leq \varepsilon$, and we choose τ so that $p_N(0) = \alpha$, where N and ε are arbitrary constants. Now by substituting $p_N(x)$ for $y(x)$ and comparing the like powers of x on both sides in (4.9), we can find the coefficients b_r and write the Eqn. (4.8) as

$$y(x) = (\alpha_1 x^{m_1} + \alpha_2 x^{m_2}) p_N(x), \quad 0 < x \leq \varepsilon. \qquad (4.10)$$

We now reduce the problem (4.1) - (4.3) to a regular boundary value problem, by finding a new boundary condition at $x = \varepsilon$. To do this we have from Eqn.(4.10),

$$y(x) \simeq \alpha_1 p(x) + \alpha_2 q(x) \qquad (4.11)$$

where $x^{m_1} p_N(x) = p(x)$ and $x^{m_2} p_N(x) = q(x)$.

Eqn. (4.11) at $x = \varepsilon$ can be written as,

$$y(\varepsilon) = \alpha_1 \, p(\varepsilon) + \alpha_2 \, q(\varepsilon) \tag{4.12}$$

We also have from Eqn. (4.11)

$$y'(\varepsilon) = \alpha_1 \, p'(\varepsilon) + \alpha_2 \, q'(\varepsilon) \tag{4.13}$$

where primes denotes the differentiation. Solving (4.12) and (4.13) for α_1 and α_2, we get

$$\alpha_1 = \frac{y(\varepsilon) \, q'(\varepsilon) - y'(\varepsilon) \, q(\varepsilon)}{p(\varepsilon) \, q'(\varepsilon) - p'(\varepsilon) \, q(\varepsilon)} \tag{4.14}$$

and

$$\alpha_2 = \frac{y'(\varepsilon) \, p(\varepsilon) - y(\varepsilon) \, p'(\varepsilon)}{p(\varepsilon) \, q'(\varepsilon) - p'(\varepsilon) \, q(\varepsilon)} \tag{4.15}$$

Since $y(0) = \alpha$, we have from Eqn. (4.11),

$$\alpha_1 \, p(0) + \alpha_2 \, q(0) = \alpha \tag{4.16}$$

using Eqns. (4.14), (4.15) and (4.16) we have

$$\frac{y(\varepsilon)q'(\varepsilon) - y'(\varepsilon)q(\varepsilon)}{p(\varepsilon)q'(\varepsilon) - p'(\varepsilon)q(\varepsilon)} \, p(0) + \frac{y'(\varepsilon)p(\varepsilon) - y(\varepsilon)p'(\varepsilon)}{p(\varepsilon)q'(\varepsilon) - p'(\varepsilon)q(\varepsilon)} \, q(0) = \alpha \tag{4.17}$$

or

$$\left[q'(\varepsilon)p(0) - p'(\varepsilon)q(0)\right] y(\varepsilon) + \left[p(\varepsilon)q(0) - q(\varepsilon)p(0)\right] y'(\varepsilon) = \alpha h(\varepsilon) \tag{4.18}$$

where $\quad h(\varepsilon) = p(\varepsilon) \, q'(\varepsilon) - p'(\varepsilon)q(\varepsilon)$.

The Eqn. (4.18) can be conveniently written

$$A_1\, y(\varepsilon) + B_1\, y'(\varepsilon) = C_1 \tag{4.19}$$

with

$$A_1 = q'(\varepsilon)p(0) - p'(\varepsilon)\, q(0)$$

$$B_1 = p(\varepsilon)\, q(0) - q(\varepsilon)\, p(0) \tag{4.20}$$

and

$$C_1 = \alpha h(\varepsilon).$$

Eqn. (4.19) gives the new boundary condition at $x = \varepsilon$. The reduced boundary value problem over $[\varepsilon, 1]$ is given by Eqn.(4.1) subject to boundary conditions (4.19) and (4.3).

In the case of non-homogeneous equation

$$y''(x)+F_1(x)y'(x)+F_2(x)y(x) = F_3(x) \tag{4.21}$$

the above procedure can be applied by making $p_N(x) = \sum_{r=0}^{N} b_r x^r$ satisfy the equation

$$y''(x)+F_1(x)y'(x)+F_2(x)y(x) = \tau\, T_N^*(x/\varepsilon)+F_3(x). \tag{4.22}$$

and obtain the coefficients b_r, by comparing the coefficients on both sides of Eqn. (4.22).

4.3 Invariant Imbedding :

We employ the method of invariant imbedding for solving the regular boundary value problem given by Eqns. (4.1), (4.19) and (4.3). By reducing the boundary value problem into a set of initial value problems, we rewrite the Eqn. (4.1) as a systems of first order equation of the form,

$$u'(x) = v(x) \tag{4.23}$$

$$-v'(x) = F_1(x)v(x)+F_2(x)u(x) \tag{4.24}$$

The corresponding boundary conditions (4.19) and (4.3) be written as,

$$A_1\ u(\varepsilon) + B_1\ v(\varepsilon) = C_1 \tag{4.25}$$

$$u(1) = \beta \tag{4.26}$$

Now let us consider a more general **first** order system given by

$$u'(x) = a(x)u(x)+b(x)v(x) + e^+(x) \tag{4.27}$$

$$x \in [\varepsilon,1]$$

$$-v'(x) = c(x)u(x)+d(x)v(x) + e^-(x) \tag{4.28}$$

with all functions $a(x)$, $b(x)$, $c(x)$, $d(x)$, $e^+(x)$ and $e^-(x)$ to be continuous in $[\varepsilon,1]$. For the general system let us write

$$u(x) = S_1(x)\ v(x) + S_2(x)u(\varepsilon)+S_3(x) \tag{4.29}$$

$$x \in [\varepsilon,1]$$

$$v(\varepsilon) = Q_1(x)\ v(x) + Q_2(x)u(\varepsilon)+Q_3(x) \tag{4.30}$$

It can be easily verified that the coefficients $S_i(x)$, $Q_i(x)$, $i = 1,2,3$ satisfy the following initial value problems

$$S_1'(x) = b(x)+[a(x)+d(x)]\ S_1(x)+c(x)S_1^2(x), \quad S_1(\varepsilon) = 0 \tag{4.31}$$

$$S_2'(x) = [a(x) + c(x)S_1(x)]\ S_2(x) \quad , \quad S_2(\varepsilon) = 1 \tag{4.32}$$

$$S_3'(x) = [a(x)+S_1(x)c(x)]\ S_3(x)+S_1(x)\bar{e}(x)+e^+(x), \quad S_3(\varepsilon) = 0 \tag{4.33}$$

$$Q_1'(x) = [d(x)+c(x)S_1(x)]\,Q_1(x) \qquad Q_1(\varepsilon) = 1 \qquad (4.34)$$

$$Q_2'(x) = [c(x)Q(x)]\ S_2(x) \qquad Q_2(\varepsilon) = 0 \qquad (4.35)$$

$$Q_3'(x) = Q_1(x)c(x)\ S_2(x) \qquad Q_3(\varepsilon) = 0 \qquad (4.36)$$

We evaluate (4.29) and (4.30) at $x = 1$, and solve (4.29), (4.30) and (4.25) as a system of three equations for the three unknowns $u(\varepsilon)$, $v(\varepsilon)$ and $v(1)$. The solution $u(x)$ for any $x \in [\varepsilon,1]$ is then derived by first finding $v(x)$ from (4.30) and using it in (4.29) to get $u(x)$.

4.4 Computational Algorithm :

To compute the solution, the computation is as follows :

Step 1 : Choose the values of N and ε and determine the shifted Chebyshev polynomial $T_N^*(x/\varepsilon)$, over the interval $(0,\varepsilon]$, ε is near to singularity. Choose τ such that $p_N(0) = \alpha$ and find the coefficients b_r in the polynomial $p_N(x)$ by solving an algebraic system resulting from making $p_N(x)$ satisfy the Eqn. (4.9).

Step 2 : Find the boundary condition (4.19) by computing the values of A_1, B_1 and C_1.

Step 3 : Integrate the initial value problems given by Eqns. (4.31)-(4.36), using efficient initial value routines from $x = \varepsilon$ to $x = 1$ to obtain the profiles S_i's and Q_i's and store them.

Step 4 : Evaluate the Eqns. (4.29) - (4.30) at $x = 1$. Using the values of $S_i(1)$ and $Q_i(1)$, $(i = 1,2,3)$ from Step 3 and

$u(1)$ from (4.26).

Step 5 : Combine the equations from Step 4 with Eqn. (4.19) (from Step 2) and solve these three equations for the unknowns $u(\varepsilon)$, $v(\varepsilon)$ and $v(1)$.

Step 6 : Compute the other values of $v(x)$, $u(x)$ for $x \varepsilon [\varepsilon, 1]$, by using the values of $u(\varepsilon)$, $v(\varepsilon)$ from Step 5, and the stored values of S_i and Q_i (for $i = 1, 2, 3$) from Step 3.

4.5 Numerical Results and Discussion :

In this section the numerical results of two model problems solved are given to demonstrate efficiency of the method. All computations were carried out on DEC-1090 Computer system.

Problem 4.1 : We consider

$$2x(1+x)\,y'' + (1+5x)y' + y = 0$$

$$y(0) = 1$$

$$y(1.5) = 1 .$$

This problem has earlier been studied by Cohen and Jones [26] by using finite difference and deferred correction approach. The analytical solution for the above problem is given by

$$y(x) = \frac{1+\sqrt{1.5}\,x^{1/2}}{(1+x)}.$$

The polynomials for $N = 5$ and $\varepsilon = 0.5$ and 0.1 are given by,

$$p_N(x) = 1.0-0.99991287x+0.9846067x^2-0.8916661x^3+0.6128445x^5$$
$$-0.2162981x^6$$

and

$$p_N(x) = 1.0-0.9999991x+0.9992441x^2-0.9968280x^3+0.9605863x^4$$
$$-0.7028661x^5$$

respectively.

Problem 4.2 : We study another problem

$$4x(1+x)y'' + (3+11x)y'+y = 0$$
$$y(0) = 1$$
$$y(1.5) = 1.$$

The analytical solution for the above problem is given by $y(x) = 1+(1.5)^{9/8}x^{1/4}/1+x.$

For our numerical experiments, we take $N = 8$, $\varepsilon = 0.5$ for which the polynomial $p_N(x)$ is given by

$$p_N(x) = 1.0-0.9999985x+0.9999175x^2-0.9984735x^3+0.9857662x^4$$
$$-0.9227079x^5+0.7374932x^6-0.4178441x^7+0.1180243x^8.$$

The numerical results for Problem 4.1 for $N = 5$ and $\varepsilon = 0.5$ and 0.1 are given in Tables 4.1 and 4.2 respectively. The computed solutions at various values of x compare very well with the analytical solution. This example has earlier been considered by Cohen and Jones [26], who have solved it using

finite difference deferred correction technique. They have used economized series expansion in the interval $[0,1]$ and obtained finite difference solution on the remaining part of the interval. By doing so they neglected the effect of singularity on the solution in the immediate neighbourhood of the singular point since the difference solution computed is far away from the singularity. Their solutions are also presented in Tables 4.1 and 4.2 and it is observed that the solutions in the viscinity of the singular point computed by invariant imbedding method are quite comparable to those of Cohen's solution obtained from economized expansion there. It has also been observed that for $\varepsilon < 1$, a comparative smaller value of N is required than for the case when $\varepsilon = 1$, for achieving the desired accuracy of the solution. Its advantage lies in solving a comparatively smaller set of algebric equations to compute the coefficients of the polynomial $p_N(x)$. This saves on both computational time and memory requirements and also minimizes loss of accuracy due to rounding errors. The computed solution which are presented in Table 4.2 are seen to be matching with the analytical solution upto atleast five places of decimal. The numerical results for Problem 4.2 for $N = 8$ and $\varepsilon = 0.5$ are given in Table 4.3 and agree with the exact solution upto five places of decimal.

TABLE 4.1

Numerical Results for the Problem 4.1

(N = 5 and ε = 0.1)

X	Imbedding Solution	Cohen's Solution [26]	Exact Solution
0.1	1.261176	1.261183	1.261180
0.2	1.289774	1.289772	1.289769
0.3	1.285252	1.285251	1.285247
0.4	1.267575	1.267574	1.267569
0.5	1.244023	1.244022	1.244017
0.6	1.217930	1.217931	1.217927
0.7	1.191003	1.191000	1.190997
0.8	1.164140	1.164139	1.164136
0.9	1.137844	1.137842	1.137839
1.0	1.112362	1.112374	1.112372
1.1	1.087870	1.087870	1.087868
1.2	1.064384	1.064303	1.064382
1.3	1.041923	1.041924	1.041923
1.4	1.020474	1.020474	1.020474
1.5	1.000000	1.000000	1.000000

TABLE 4.2

Numerical Results for the Problem 4.1

(N = 5, and ε = 0.5)

X	Imbedding Solution	Cohen's Solution [26]	Exact Solution
0.5	1.244025	1.244022	1.244017
0.6	1.217933	1.217931	1.217927
0.7	1.191010	1.191000	1.190997
0.8	1.164138	1.164139	1.164136
0.9	1.137846	1.137842	1.137839
1.0	1.112376	1.112374	1.112372
1.1	1.087872	1.087870	1.087868
1.2	1.064384	1.064383	1.064382
1.3	1.041926	1.041924	1.041923
1.4	1.020474	1.020474	1.020474
1.5	1.000000	1.000000	1.000000

TABLE 4.3

Numerical Results for the Problem 4.2

($N = 8$, and $\varepsilon = 0.5$)

X	Imbedding Solution	Exact Solution
0.5	1.4265032	1.426502
0.6	1.3705673	1.370566
0.7	1.3175152	1.317515
0.8	1.2677009	1.267701
0.9	1.2211408	1.221141
1.0	1.1777007	1.177701
1.1	1.1371838	1.137184
1.2	1.0993700	1.099369
1.3	1.0640368	1.064037
1.4	1.0309788	1.030979
1.5	1.0000000	1.000000

CHAPTER 5

MODIFIED FOURTH ORDER FINITE DIFFERENCE METHOD FOR LINEAR SINGULAR BOUNDARY VALUE PROBLEMS

5.1 Introduction: Most of our attempts towards the development of numerical techniques for linear singular boundary value problems mentioned in the previous chapters are based on the removal of singularity by making use of expansion procedures in the vicinity of the singularity. However the method of finite differences is another practical method suited to the numerical solution of singular two point boundary value problems. However for some problems, it may sometimes be difficult or even not possible to obtain the series solution in the neighbourhood of the singularity. In such cases, one may need a direct method to solve singular boundary value problems. The method of finite differences, which is quite popular for solving boundary value problems, can be one such direct approach to tackle these problems.

Finite difference methods for singular problems have been studied by several authors namely Jamet [50], Gustaffsson [47], Chawla [21], Deodel and Reddien [37], Russell and Shampine [83], deHoog and Weiss [29], and Brabston and Keller [16]. Chawla [21] has discussed the construction of three point finite difference approximations and their convergence under appropriate conditions for a class of singular two point boundary value problems. This has been done by establishing a certain identity based on a general mesh, from which various methods are derived. Also

Russell and Shampine [83] have used the traditional second order finite difference, patch bases and collocation methods for singular boundary value problems. Recently Deodel and Reddien [37] have constructed some finite difference schemes for these problems and showed how these methods can be viewed as a special type of collocation scheme.

The object of this chapter is to present a modified fourth order finite difference method to solve a certain class of linear singular boundary value problem. The original differential equation is modified at the singular point. The main feature of the modified difference scheme is that it leads to the tridiagonal system of equations which has been treated by discrete invariant imbedding method. The Numerical experiments for the model problems have been given to illustrate the method.

5.2 Difference Method :

We consider a certain class of singular boundary value problems given by

$$\frac{d^2y}{dx^2} + \frac{K}{x}\frac{dy}{dx} - q(x)y(x) = f(x), \quad 0 < x < 1 \tag{5.1}$$

with $K \geq 1$ and subject to boundary conditions

$$y'(0) = 0 \tag{5.2}$$

$$y(1) = \beta \tag{5.3}$$

As Jamet [50] has shown that for the Eqn. (5.1), the derivative boundary condition is imposed due to nature of the physical

situation of the problem. Due to singularity at $x = 0$, we need modification of the problem near the singular point. We present a modified fourth order finite difference method, which leads to a tridiagonal system.

We divide the interval $0 = x_0 < x_1 < x_2 \dots < x_n = 1$ into n equal parts with uniform mesh size $x_i - x_{i-1} = h$, where h is the mesh size. By using a fourth order difference method and employing central difference formulae for the first and second order derivatives [42] , we may write Eqn. (5.1) as,

$$\frac{1}{h^2}\{\delta^2 - \frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 - \frac{1}{560}\delta^8 + \dots\}y_i +$$

$$+ \frac{K}{hx_i}\{\mu\delta - \frac{1}{6}\mu\delta^3 + \frac{1}{30}\mu\delta^5 + \dots\}y_i$$

$$- q_i y_i = f_i, \quad i = 1, 2, \dots, n-1 \tag{5.4}$$

where $y_i = y(x_i)$.

Rewriting Eqn. (5.4) in a compact form,

$$\frac{1}{h^2}\{\delta^2 - \frac{1}{12}\delta^4\} y_i + \frac{K}{hx_i}\{\mu\delta - \frac{1}{6}\mu\delta^3\}y_i - q_i y_i = f_i + E_i \tag{5.5}$$

where $E_i = -\frac{1}{h^2}\{\frac{1}{90}\delta^6 + \dots\} y_i - \frac{K}{hx_i}\{\frac{1}{30}\mu\delta^5 + \dots\} y_i$ (5.6)

and $E_i = O(h^4)$ (5.7)

Eqn. (5.5) is a fourth order finite difference method which is not tridiagonal due to the presence of the differences $\mu\delta^3 y_i$ and $\delta^4 y_i$ in the left hand side of the equation. To make

Eqn. (5.5) a tridiagonal system, we make the tridiagonal estimate of $\mu\delta^3 y_i$ and $\delta^4 y_i$ upto order five and six respectively.

At the singular point $x = 0$, we modify Eqn.(5.1) as,

$$(1+K)y''(x) - q(x)y(x) = f(x), \quad x = x_o \tag{5.8}$$

For Eqn. (5.8), we apply the above mentioned fourth order finite difference formulae at $x = x_o$ ($x_o = 0$) and obtain

$$\frac{(1+K)}{h^2}\{\delta^2 - \frac{1}{12}\delta^4\} y_o - q_o y_o = f_o + H_o \tag{5.9}$$

where $H_o = \{-\frac{1}{h^2} \cdot \frac{1}{90}\delta^6 + \frac{1}{h^2} \cdot \frac{\delta^8}{560} \ldots\} y_o$.

Differentiating Eqn. (5.8) twice with respect to x yields,

$$(1+K)y^{iv}(x) - q''(x)y(x) - 2q'(x)y'(x) - qy''(x) = f''(x), \quad x = x_o$$

or

$$y^{iv}(x) = \frac{1}{(1+K)}\{q(x)y''(x) + 2q'(x)y'(x) + q''(x)y(x) + f''(x)\}, \quad x = x_o$$

or

$$y^{iv}(x_o) = \frac{1}{(1+K)}\{q(x_o)y''(x_o)\} + \frac{2}{(1+K)}q'(x_o)y'(x_o) + \frac{q''(x_o)}{(1+K)}y(x_o) + \frac{f''(x_o)}{(1+K)} \tag{5.10}$$

or

$$\delta^4 y(x_o) = \frac{h^3}{(1+K)}q(x_o)\,\delta^2 y(x_o) + \frac{2h^3}{(1+K)}q'(x_o)\,\mu\delta y(x_o) + \frac{h^4 q''(x_o)}{(1+K)}y(x_o) + \frac{h^4 f''(x_o)}{(1+K)} + G_i$$

$$\text{where } G_i = O(h^6) \tag{5.11}$$

Substituting Eqn. (5.11) in (5.9) we get

$$\frac{(1+K)}{h^2}\delta^2 y_o - \frac{(1+K)}{12h^2}\{\frac{h^2}{(1+K)} q(x_o)\,\delta^2 y(x_o) + \frac{2h^3}{(1+K)} q'(x_o)\,\mu\delta y(x_o)$$

$$+ \frac{h^4 q''(x_o)}{(1+K)}\, y(x_o) + \frac{h^4 f''(x_o)}{(1+K)}\} - q_o y_o + A_i = f_i \qquad (5.12)$$

where $A_i = O(h^6)$

By neglecting the truncation error term and after some algebra, we get

$$[1 - \frac{q_o h^2}{12(1+K)} - \frac{h^3 q_o'}{12(1+K)}]y_1 - [\frac{5h^2 q_o}{6(1+K)} + \frac{h^4 q_o''}{12(1+K)} + 2]\,y_o$$

$$+ [1 - \frac{h^2 q_o}{12(1+K)} + \frac{h^3 q_o'}{12(1+K)}]\,y_{-1} = \frac{h^2 f_o}{(1+K)} + \frac{h^4}{12} f_o'' \qquad (5.13)$$

where $q_o = q(x_o)$, $q_o' = q'(x_o)$, $f_o = f(x_o)$ and $f_o' = f'(x_o)$.

Using Eqn. (5.2) and (5.13), Eqn. (5.13) can be written in a compact form,

$$(L_o + N_o)y_1 - M_o y_o = P_o \qquad (5.14)$$

where,

$$L_o = -\frac{h^3 q_o'}{12(1+K)} - \frac{h^2 q_o}{12(1+K)} + 1 \qquad (5.15)$$

$$M_o = \frac{5h^2 q_o}{6(1+K)} + \frac{h^4 q_o''}{12(1+K)} + 2 \qquad (5.16)$$

$$N_o = \frac{h^3 q_o'}{12(1+K)} - \frac{h^2 q_o}{12(1+K)} + 1 \tag{5.17}$$

and

$$P_o = \frac{h^2 f_o}{(1+K)} + \frac{h^4}{12} \frac{f_o''}{(1+K)} \tag{5.18}$$

Differentiating Eqn.(5.1) with respect to x, we get the tridiagonal estimate of $\mu\delta^3 y_i$ $(i = 1,2,\ldots,n-1)$ as

$$y_i''' + \frac{K}{x} y_i'' - \frac{K}{x^2} y_i' - q_i' y_i - q_i y_i' = f_i' \;, \quad (i = 1,2,\ldots,n-1)$$

or $$\mu\delta^3 y_i + \frac{hK}{x_i} \delta^2 y_i - \frac{Kh^2}{x_i^2} \mu\delta y_i - h^3 q_i' y_i - h^2 q_i \mu\delta y_i = h^3 f_i'$$

$$(i = 1,2,\ldots,n-1)$$

or $$\mu\delta^3 y_i = -\frac{Kh}{x_i} \delta^2 y_i + h^2\left(\frac{K}{x_i^2} + q_i\right) \mu\delta y_i$$

$$+ h^3 q_i' y_i + h^3 f_i' + O(h^5) \tag{5.19}$$

Similarly differentiating Eqn.(5.1) twice with respect to x, we get the tridigonal estimate of $\delta^4 y_i$ as

$$\delta^4 y_i = h^2\left(\frac{K^2}{x_i^2} + \frac{K}{x_i^2} + q_i\right) \delta^2 y_i$$

$$+ h^3\left(2q_i' + \frac{Kq_i}{x_i} - \frac{2K}{x_i^3} - \frac{2K^2}{x_i^3}\right) \mu\delta y_i$$

$$+ h^4\left(q_i'' + \frac{K}{x_i} q_i' - \frac{Kq_i}{x_i^2}\right) y_i + h^4\left(f_i'' - \frac{K}{x_i} f_i' + \frac{K}{x_i^2} f_i\right)$$

$$+ O(h^6) \tag{5.20}$$

Using Eqn. (5.19) and (5.20) into Eqn. (5.5) and rearranging the terms we get a tridiagonal system

$$L_i\, y_{i+1} - M_i y_i + N_i\, y_{i-1} = P_i,\quad i = 1,2,\ldots,n-1 \tag{5.21}$$

where

$$L_i = 1 + \frac{Kh}{2x_i} + \frac{h^2}{12}\left(\frac{K^2}{x_i^2} - \frac{K}{x_i^2} - q_i\right) + \frac{h^3}{24}\left(\frac{2K}{x_i^3} - 2q_i' - \frac{Kq_i}{x_i}\right) \tag{5.22}$$

$$M_i = \frac{h^4}{12}\left(q_i'' + \frac{K}{x_i}\, q_i' - \frac{K}{x_i^2}\, q_i\right) + \frac{h^2}{6}\left(5q_i + \frac{K^2}{x_i^2} - \frac{K}{x_i^2}\right) + 2 \tag{5.23}$$

$$N_i = 1 - \frac{hK}{2x_i} + \frac{h^2}{12}\left(\frac{K^2}{x_i^2} - \frac{K}{x_i^2} - q_i\right) - \frac{h^3}{24}\left(\frac{2K}{x_i^3} - 2q_i' - \frac{Kq_i}{x_i}\right) \tag{5.24}$$

and

$$P_i = h^2 f_i + \frac{h^4}{12}\left(f_i'' + \frac{K}{x_i}\, f_i' + \frac{K}{x_i^2}\, f_i\right) \tag{5.25}$$

Eqns. (5.14) and (5.21) contribute a difference system of n equations with n unknowns.

5.3 Computational Method :

To solve the tridiagonal system we make use of the method of invariant imbedding [7]. We seek a difference relation of the form,

$$y_i = W_i y_{i+1} + T_i,\quad i = 0,1,2,\ldots,n-1 \tag{5.26}$$

where W_i and T_i correspond to $W(x_i)$ and $T(x_i)$ and are to be determined.

Using Eqn. (5.26) in (5.21), we have

$$L_i y_{i+1} - M_i y_i + N_i(W_{i-1}y_i + T_{i-1}) = P_i$$

or

$$L_i y_{i+1} + (N_i W_{i-1} - M_i) y_i = P_i - N_i T_{i-1}.$$

$$y_i\,[N_i W_{i-1} - M_i] = -L_i y_{i+1} + [P_i - N_i T_{i-1}]$$

or

$$y_i = \frac{L_i}{(M_i - N_i W_{i-1})}\, y_{i+1} + \frac{[P_i - N_i T_{i-1}]}{(N_i W_{i-1} - M_i)} \qquad (5.27)$$

Comparing Eqn. (5.27) with Eqn. (5.26), we see tha t the recurrence relations for W_i and T_i for $i = 1, 2, \ldots, n-1$ are obtained as

$$W_i = \frac{L_i}{(M_i - N_i W_{i-1})} \qquad (5.28)$$

and

$$T_i = \frac{P_i - N_i T_{i-1}}{(N_i W_{i-1} - M_i)} \qquad (5.29)$$

To solve the recurrence relations for W_i and T_i, we need to know the initial conditions for W_o and T_o. These initial values can be easily obtained as,

$$W_o = \frac{(L_o + N_o)}{M_o} \qquad (5.30)$$

and

$$T_o = -\frac{P_o}{M_o} \tag{5.31}$$

where L_o, M_o, N_o and P_o are given by Eqns. (5.15) - (5.18). Using the initial values, we compute W_i and T_i for $i = 1, 2, \ldots, n-1$, from Eqns. (5.28) and (5.29) in the forward sweep manner and then obtain the solutions y_i in the backward process using the Eqn. (5.26).

5.4 Numerical Results and Discussion :

In this section the numerical results of the model problems solved are presented

Problem 5.1 : We solve

$$y'' + \frac{2}{x} y' - 4y = -2$$

$$y'(0) = 0$$

$$y(1) = 5.5$$

This problem has earlier been solved by Russell and Shampine [83], which has the exact solution

$$y(x) = \frac{1}{2} + \frac{5 \sinh 2x}{x \sinh 2}$$

Problem 5.2 : We solve another model, a non-homogeneous equation

$$-y'' - \frac{2}{x} y' + (1-x^2)y = 7-2x^2+x^4$$

$$y'(0) = 0$$

$$y(1) = 0.$$

This is the model problem used by K. Eriksson and V. Thomee [39] and has the exact solution $y(x) = 1-x^2$.

The computational results for the Problem 5.1 for different mesh sizes are given in Table 5.1. It is evident from the results that the modified finite difference method works well and the solutions are quite comparable with the exact solution. The results indicate that near the singularity one may not need a very small mesh size due to the modified scheme. The maximum error between the approximate solution and the computed solution at the mesh points for different values of h are given in Table 5.2. Also comparison of the maximum errors with regard to other methods is presented in Table 5.2. It is observed that the fourth order finite difference scheme gives better accuracy than other methods.

The results for the Problem 5.2 are given in Table 5.3. The results indicate the efficiency of the method for the non-homogeneous problem also.

TABLE 5.1

Results for the Problem 5.1

x	$N = \frac{1}{h}$ 10	20	40	60	Exact Solution
0.0	3.257304	3.257213	3.257203	3.257199	–
0.1	3.275707	3.275629	3.275622	3.275618	3.275624
0.2	3.331380	3.331325	3.331319	3.331316	3.331322
0.3	3.425684	3.425643	3.425639	3.425636	3.425641
0.4	3.560894	3.560864	3.560861	3.560859	3.561863
0.5	3.740294	3.740271	3.740269	3.740268	3.740271
0.6	3.968262	3.968246	3.968244	3.968243	3.968246
0.7	4.250404	4.250393	4.250391	4.250390	4.250393
0.8	4.593712	4.593705	4.593703	4.593704	4.593706
0.9	5.006769	5.006766	5.006765	5.006766	5.006766

TABLE 5.2

Maximum Error* in the Solution for the Problem 5.1

$N = \frac{1}{h}$	Russell and Shampine finite Diff. method [83]	Russell and Shampine Patch bases [83]	Present method
4	2.12×10^{-1}	2.02×10^{-1}	1.56×10^{-3}
9	5.05×10^{-2}	4.09×10^{-2}	1.20×10^{-4}
16	1.80×10^{-2}	1.30×10^{-2}	1.70×10^{-5}
25	8.02×10^{-3}	5.33×10^{-3}	3.01×10^{-6}
64	1.43×10^{-3}	8.14×10^{-4}	1.67×10^{-6}

*Difference between the approximate analytical solution and the computed solution.

TABLE 5.3

Results for the Problem 5.3

x	$N = \frac{1}{h}$: 10	20	40	60	Exact Solution
0.0	1.023449	1.005877	1.001470	1.000652	1.000000
0.1	0.9902004	0.9900503	0.9900121	0.9900040	0.9900000
0.2	0.9601876	0.9600467	0.9600112	0.9600037	0.9600000
0.3	0.9101648	0.9100408	0.9100097	0.9100033	0.9100000
0.4	0.8401344	0.8400330	0.8400080	0.8400076	0.840000
0.5	0.7500991	0.7500242	0.7500060	0.7500017	0.750000
0.6	0.6400624	0.6400150	0.6400039	0.6400008	0.640000
0.7	0.5100286	0.5100066	0.5100018	0.5100001	0.510000
0.8	0.3600027	0.3600003	0.3600002	0.3599996	0.360000
0.9	0.1899909	0.1899975	0.1899994	0.1899995	0.1900001

CHAPTER VI

DIFFERENCE METHOD FOR NONLINEAR SINGULAR PROBLEMS

6.1 Introduction: The object of this chapter is to extend the finite difference method described in Chapter V to non-linear singular boundary value problems. We shall consider a class of non-linear problems of the following form :

$$y''(x) + \frac{m}{x} y'(x) - q(x)y(x) = f(x,y) \qquad (6.1)$$

subject to the boundary conditions

$$y'(0) = 0 \qquad (6.2)$$

$$y(1) = \beta \qquad (6.3)$$

where $m \geq 1$ and β is given constant. We assume that (i) $f(x,y)$ is continuous (ii) $\frac{\partial f}{\partial y}$ exists and is continuous and $\frac{\partial f}{\partial y} \geq 0$. The application of finite difference methods to these problems has been discussed by some authors namely Jamet [50], Deodel and Reddien [37]. A three point finite difference scheme has been proposed by Russell and Shampine [83] with Newtons iteration procedure for solving non-linear problems.

In this chapter we have presented a method based on finite difference technique for non-linear singular boundary value problems. The quasilinearization technique, originally developed by Bellman and Kalaba [12], has been used to reduce

the given non-linear problem to a sequence of linear problems. The fourth order finite difference method, similar to the one described in the previous chapter, has been applied to solve the linear problems. Some model problems have been solved to demonstrate the efficiency of the method. The comparison of numerical results is also made with other methods.

6.2 Quasilinearization :- In the Quasilinearization technique, instead of being solved directly, the non-linear differential equation, is solved recurssively by a sequence of linear differential equations. The main advantage of this method is that if the procedure converges, it converges **quadratically** to the solution of the original problem. Quadratic convergence means that the error in the (K+1)th iteration is proportional to the square of the error in Kth iteration. The linear equation is obtained by using the first and second term in the Taylor's series expansion of the original non-linear differential equation.

Consider Eqn. (6.1) with boundary conditions (6.2), (6.3). We choose a reasonable initial approximation for the function $y(x)$ in $f(x,y)$, call it as $y^{(0)}(x)$ and expand f around the function $y^{o}(x)$, we have

$$f(x,y^{(1)}) = f(x,y^{(o)}) + (y^{(1)}-y^{(o)}) \left.\frac{\partial f}{\partial y}\right|_{(x,y^{(0)})} + \cdots \tag{6.4}$$

Or, in general we can write for $k = 0,1,2,\ldots$

$$f(x,y^{(k+1)}) = f(x,y^{(k)}) + (y^{(k+1)}-y^{(k)})\left.\frac{\partial f}{\partial y}\right|_{(x,y^{(k)})} + \cdots \qquad (6.5)$$

Eqn. (6.1) can be written as

$$y''^{(k+1)} + \frac{m}{x} y'^{(k+1)} - q(x)y^{(k+1)} = f(x,y^{(k)})$$

$$+ (y^{(k+1)} - y^{(k)})\left.\frac{\partial f}{\partial y}\right|_{(x,y^{(k)})} \qquad (6.6)$$

$$k = 0,1,2,\ldots$$

subject to the boundary conditions

$$y'^{(k+1)}(0) = 0 \qquad (6.7)$$

$$y^{(k+1)}(1) = \beta \qquad (6.8)$$

Let us re-write the Eqn. (6.6) in the following form

$$y''^{(k+1)} + \frac{m}{x} y'^{(k+1)} - r^{(k)}(x)y^{(k+1)} = F^{(k)}(x) \qquad (6.9)$$

where

$$r^{(k)}(x) = q(x) + \left.\frac{\partial f}{\partial y}\right|_{(x,y^{(k)})} \qquad (6.10)$$

$$F^{(k)}(x) = f(x,y^{(k)}) - y^{(k)}\left.\frac{\partial f}{\partial y}\right|_{(x,y^{(k)})} . \qquad (6.11)$$

and $k = 0,1,2,\ldots$.

6.3 Difference Method : - In order to solve the system of linear singular boundary value problem given by Eqn. (6.9) subject to Eqns. (6.7) - (6.8), we use the fourth order finite

difference method described in the **previous chapter.** Due to the singularity at $x = 0$ we need to modify the problem at $x = 0$. As usual, we divide the interval $[0,1]$ into N equal sub-interval with fixed step length h such that $0 = x_0 < x_1 < \cdots < x_N = 1$. By employing central difference formulae for the first and second order derivatives and taking upto fourth order terms we get the difference equation for (6.9) as

$$\frac{1}{h^2}\left[\delta^2 - \frac{1}{12}\delta^4\right] y_i^{(k+1)} + \frac{m}{x_i}\left[\mu\delta - \frac{1}{6}\mu\delta^3\right] y_i^{(k+1)}$$

$$- r_i^{(k)} y_i^{(k+1)} = F_i^{(k)} + E_i \qquad (6.12)$$

where $r_i^{(k)} = r^{(k)}(x_i)$ and $F_i^{(k)} = F^{(k)}(x_i)$ and $y_i^{(k+1)} = y^{(k+1)}(x_i)$ and

$$E_i = -\frac{1}{h^2}\left\{\frac{1}{90}\delta^6 + \cdots\right\} y_i^{(k+1)} - \frac{m}{hx_i}\left\{\frac{1}{30}\mu\delta^5 + \cdots\right\} y_i^{k+1} \qquad (6.13)$$

with $i = 1,2,\ldots,N-1$.

and $k = 0,1,2,\ldots$.

As discussed in Chapter V, at the singular point $x = x_0$, the modified differential equation can be written as follows

$$(1+m)\, y''^{(k+1)}(x) - r^{(k)}(x)\, y^{(k+1)}(x) = F^{(k)}(x), \quad x = x_0,$$

$$k = 0,1,2,\ldots \qquad (6.14)$$

Re-writing Eqn. (6.14) we have

$$y''^{(k+1)}(x) - \frac{r^{(k)}(x)}{(1+m)} y^{(k+1)}(x) = \frac{F^{(k)}(x)}{(1+m)} \tag{6.15}$$

We will now employ the fourth order finite difference method at $x = 0$ for this modified equation (6.15). Then we get, a difference equation at $x = x_o (= 0)$ as

$$\frac{1}{h^2} [\delta^2 - \frac{1}{12}\delta^4] y_o^{(k+1)} - \frac{r^{(k)}(x)}{(1+m)} y_o^{(k+1)} = \frac{F_o^{(k)}}{(1+m)} + E_o \tag{6.16}$$

where $\quad E_o = -\frac{1}{h^2}[\frac{\delta^6}{90} + \ldots\ldots] y_o^{(k+1)}.$

To make the equations (6.12) and (6.16) as tridiagonal system, we first make the tridiagonal estimates for $\mu\delta^3 y_i^{(k+1)}$, $\delta^4 y_i^{(k+1)}$ and $\delta^4 y_o^{(k+1)}$ as follows. Differentiating Eqn. (6.15) twice we get at $x = x_o$,

$$y'''^{(k+1)}(x) - \frac{r'^{(k)}(x)}{(1+m)} y^{(k+1)}(x) - \frac{r^{(k)}(x)}{(1+m)} y'^{(k+1)}(x)$$

$$= \frac{F'^{(k)}(x)}{(1+m)}, \quad x = x_o$$

$$y^{iv(k+1)}(x) - \frac{r''^{(k)}(x)}{(1+m)} y^{(k+1)}(x) - \frac{r'^{(k)}(x)}{(1+m)} y''^{(k+1)}(x)$$

$$- \frac{r'^{(k)}(x)}{(1+m)} y'^{(k+1)}(x) - \frac{r^{(k)}(x)}{(1+m)} y''^{(k+1)}(x)$$

$$= \frac{F''^{(k)}(x)}{(1+m)}, \quad x = x_o \tag{6.17}$$

The tridiagonal estimate of $\delta^4 y_0^{(k+1)}$ $(k = 0,1,2,\ldots)$ for Eqn. (6.17) yields,

$$\delta^4 y_0^{(k+1)} = h^2\left(\frac{r_0^{(k)}}{(1+m)}\right)\delta^2 y_0^{(k+1)} + h^3\left(\frac{2r_0'^{(k)}}{(1+m)}\right)\mu\delta y_0^{(k+1)}$$

$$+ h^4\left(\frac{r_0''^{(k)}}{(1+m)}\right)y_0^{(k+1)} + h^4\left(\frac{F_0''^{(k)}}{(1+m)}\right) + O(h^6),$$

$$k = 0,1,2,\ldots \tag{6.18}$$

Substituting Eqn. (6.18) in (6.16) and neglecting the error terms, after some manipulations we get,

$$\left[1 - \frac{h^2}{12}\frac{r_0^{(k)}}{(1+m)} - \frac{h^3}{12}\frac{r_0'^{(k)}}{(1+m)}\right]y_1^{(k+1)}$$

$$- \left[2 + \frac{5h^2}{6}\left(\frac{r_0^{(k)}}{(1+m)}\right) + \frac{h^4}{12}\left(\frac{r_0''^{(k)}}{(1+m)}\right)\right] y_0^{(k+1)}$$

$$+ \left[1 - \frac{h^2}{12}\frac{r_0^{(k)}}{(1+m)} + \frac{h^3}{12}\frac{r_0'^{(k)}}{(1+m)}\right] y_{-1}^{(k+1)}$$

$$= \frac{h^2 F_0^{(k)}}{(1+m)} + \frac{h^4}{12}\frac{F_0''^{(k)}}{(1+m)} \quad k = 0,1,2,\ldots \tag{6.19}$$

By using Eqns. (6.7) and (6.19), we write Eqn. (6.19) in a compact form as

$$(A_0 + C_0)\; y_1^{(k+1)} - B_0 y_0^{(k+1)} = D_0 \tag{6.20}$$

where,

$$A_o = 1 - \frac{h^2}{12}\frac{r_o^{(k)}}{(1+m)} - \frac{h^3}{12}\frac{r_o'^{(k)}}{(1+m)} \qquad (6.21)$$

$$B_o = 2 + \frac{5h^2}{6}\frac{r_o^{(k)}}{(1+m)} + \frac{h^4}{12}\frac{r_o''^{(k)}}{(1+m)} \qquad (6.22)$$

$$C_o = 1 - \frac{h^2}{12}\frac{r_o^{(k)}}{(1+m)} + \frac{h^3}{12}\frac{r_o'^{(k)}}{(1+m)} \qquad (6.23)$$

and

$$D_o = \frac{h^2 F_o^{(k)}}{(1+m)} + \frac{h^4}{12}\frac{F_o''^{(k)}}{(1+m)} \qquad (6.24)$$

for $k = 0, 1, 2, \ldots$.

Again differentiating Eqn. (6.9) twice with respect to x, and neglecting the error terms, we get the tridiagonal estimates of $\mu\delta^3 y_i$ and $\delta^4 y_i$ $(i = 1, 2, \ldots, N-1)$ as,

$$\mu\delta^3 y_i^{(k+1)} = -\frac{h}{x_i}\,\delta^2 y_i^{(k+1)} - h^2\left(-\frac{M}{x_i^2} - r_i^{(k)}\right)\mu\delta y_i^{(k+1)}$$

$$+ h^3 r_i'^{(k)} y_i^{(k+1)} + h^3 F_i'^{(k)} + O(h^5)$$

$$k = 0, 1, 2, \ldots \qquad (6.25)$$

and $$\delta^4 y_i = h^2\left(\frac{m^2}{x_i^2} + \frac{m}{x_i^2} + r_i^{(k)}\right)\delta^2 y_i^{(k+1)}$$

$$+ h^3\left(2r_i'^{(k)} + \frac{m}{x_i} r_i^{(k)} - \frac{2m}{x_i^3} - \frac{2m^2}{x_i}\right)\mu\delta y_i^{(k+1)}$$

$$+ h^4\left(r_i''^{(k)} + \frac{m}{x_i} r_i'^{(k)} - \frac{m r_i^{(k)}}{x_i^2}\right) y_i^{(k+1)}$$

$$+ h^4\left(F_i''^{(k)} - \frac{m}{x_i} F_i'^{(k)} + \frac{m}{x_i^2} F_i^{(k)}\right) + O(h^6) \qquad (6.26)$$

$$k = 0, 1, 2, \ldots .$$

Substituting Eqns. (6.25) - (6.26) in (6.12) and rearranging the terms we get a tridiagonal system (by neglecting the error term E_i) as,

$$A_i y_{i+1}^{(k+1)} - B_i y_i^{(k+1)} + C_i y_{i-1}^{(k+1)} = D_i, \quad i = 1, 2, \ldots, N-1$$

$$k = 0, 1, 2, \ldots \qquad (6.27)$$

where

$$A_i = 1 + \frac{h}{2}\frac{m}{x_i} + \frac{h^2}{12}\left(\frac{m^2}{x_i^2} - \frac{m}{x_i^2} - r_i^{(k)}\right)$$

$$+ \frac{h^3}{24}\left(\frac{2m}{x_i^3} - 2r_i'^{(k)} - \frac{mr_i^{(k)}}{x_i}\right) \qquad (6.28)$$

$$B_i = 2 + \frac{h^2}{6}\left(5r_i + \frac{m^2}{x_i^2} - \frac{m}{x_i^2}\right)$$

$$+ \frac{h^4}{12}\left(r_i''^{(k)} + \frac{mr_i'^{(k)}}{x_i} - \frac{mr_i^{(k)}}{x_i^2}\right) \qquad (6.29)$$

$$C_i = 1 - \frac{h}{2}\frac{m}{x_i} + \frac{h^2}{12}\left(\frac{m^2}{x_i^2} - \frac{m}{x_i^2} - r_i^{(k)}\right)$$

$$- \frac{h^3}{24}\left(\frac{2m}{x_i^3} - 2r_i'^{(k)} - \frac{mr_i^{(k)}}{x_i}\right) \qquad (6.30)$$

and

$$D_i = h^2 F_i^{(k)} + \frac{h^4}{12}\left(F_i'' + \frac{m}{x_i} F_i'^{(k)} + \frac{k}{x_i^2} F_i^{(k)}\right) \qquad (6.31)$$

where $r^{(k)}(x)$ and $F^{(k)}(x)$ are defined by Eqns. (6.10) and (6.11) respectively.

We observe that Eqns. (6.20) and (6.27) produce a tridiagonal system of n equations with n unknowns, which can be solved by the methods discussed earlier. The approximate solution values, at each stage of the iteration $(k = 0,1,2,\ldots)$ are computed till the convergence criteria $|y_i^{(k+1)} - y_i^{(k)}| < EPS$, where EPS, is given value, is satisfied.

6.4 Numerical Results and Discussion :

In this section, some physical model problems solved are presented. All computations were done on DEC-1090 computer system with single precision arithmetic.

Problem 6.1 : We consider the problem arising in Astronomy, the equilibrium of isothermal gas spheres can be described by

$$y''(x) + \frac{2}{x}\, y'(x) + y^5 = 0$$

with boundary conditions

$$y'(0) = 0$$

$$y(1) = \sqrt{3/2}$$

which has a exact solution $y(x) = 1/\sqrt{1 + \frac{1}{3}x^2}$. This problem is stated in Russell and Shampine [83] , Hoog and Weiss [29] and Rentrop [53] .

Problem 6.2 : We solve

$$y''(x) + \frac{1}{x}\, y'(x) + e^{y(x)} = 0$$

with boundary conditions

$$y'(0) = 0$$

$$y(1) = 0$$

This problem has earlier been discussed by Russell and Shampine [83]. The exact solutions are $y(x) = 2\log\left(\frac{B+1}{Bx^2+1}\right)$, where $B = 3 \pm 2\sqrt{2}$.

Problem 6.3 : The equation for one dimensional heat conduction with non-linear heat generation is given by

$$y''(x) = -\frac{1}{x}\, y'(x) - \lambda e^{y(x)}$$

with boundary conditions

$$y'(0) = y(1) = 0$$

where λ : heat generation constant, $0 < \lambda \leq 0.8$

y : temperature distribution.

This problem possesses a numerical singularity at $x = 0$. This problem has been considered earlier by NA [67].

Problem 6.4 : As a last example, we solve

$$y''(x) + \frac{a}{x}\, y'(x) = \varphi^2 y(x)\, \exp\left[\frac{\gamma\beta(1-y(x))}{1+\beta(1-y(x))}\right]$$

subject to boundary conditions $y'(0) = y(1) = 0$.

y : dimensionless concentration

a : structure of catalyst particle, $a = 2$ spherical

β, γ, φ : chemical constants.

This problem is studied by Rentrop [67], for different values of β, γ and φ.

The numerical results for problem 6.1 for different values of mesh size h are presented in Table 6.1. These solutions correspond to the iteration index $k = 4$ by taking $y_0 = 0$ as the initial approximation. The iterations were stopped by satisfying the absolute error criterion $|y_i^{(k+1)}-y_i^{(k)}| \leq 10^{-5}$ for all i. As it is apparant from the table, the results converge to the exact solution. The comparison of the computed solution of this program for $h = 1/64$ with other methods is given in Table 6.2. It can be observed that our solutions compare well with the solutions obtained by other methods. It can also be noticed that the solution near the singular point is not affected much due to the removal of the singularity at $x = 0$.

The numerical results for Problem 6.2 for different value of h are given in Table 6.3. These results correspond to the iteration index $k = 3$ and $y_0 = 0$ as the initial approximation. The comparison of the computer solutions obtained by different methods is presented in Table 6.4. It can again be observed that the results agree well with the smaller solution, which is the exact solution with the value of B equal to $3-2\sqrt{2}$. The numerical results for problem 6.3 for $\lambda = 0.8$ are given in Table 6.5. These solutions correspond to $k = 4$ and $y_0 = 0$.

The numerical results for Problem 6.4 are given in Tables 6.6 and 6.7. Table 6.6 presents computed solutions for $\beta = \gamma = \varphi = 1$ and the computed solutions for $\beta = 0.05$, $\gamma = 20$ and $\varphi = 6$ are given in Table 6.7. The value of a in both these cases has been taken equal to 2. These solutions correspond to $y_o = 0$ and $k = 4$ satisfying the stopping criterion

$$|y_i^{(k+1)} - y_i^{(k)}| \leq 10^{-6} \text{ for all } i.$$

The solutions are seen to compare well with the solutions obtained by Rentrop [67].

Table 6.1

Numerical Results for Problem 6.1

x	N = $\frac{1}{h}$			
	10	20	40	60
0.0	0.9976150	0.9993991	0.9998491	0.9999315
0.1	0.9976565	0.9981592	0.9982917	0.9983156
0.2	0.9927323	0.9932253	0.9933547	0.9933780
0.3	0.9846899	0.9851631	0.9852869	0.9853090
0.4	0.9737577	0.9742001	0.9743154	0.9743359
0.5	0.9602305	0.9606300	0.9607338	0.9607521
0.6	0.9444484	0.9447922	0.9448813	0.9448968
0.7	0.9267758	0.9270509	0.9271218	0.9271342
0.8	0.9075811	0.9077749	0.9078247	0.9078335
0.9	0.8872205	0.8873219	0.8873479	0.8873525

Table 6.2

Comparison Table for Problem 6.1

$$(h = \frac{1}{64})$$

x	Patch bases [83]	Finite Difference [83]	Our Method	Exact Solution
0.000	0.99992	1.00000	0.9999372	1.0000000
0.125	0.99737	0.99742	0.9973843	0.9974060
0.250	0.98971	0.98976	0.9897231	0.9897433
0.375	0.97733	0.97737	0.9773373	0.9773556
0.500	0.96075	0.96078	0.9607530	0.9607689
0.625	0.94062	0.94064	0.9406213	0.9406342
0.750	0.91765	0.91767	0.9176537	0.9176629
0.875	0.89257	0.89256	0.8925647	0.8925696

Table 6.3

Numerical Results for Problem 6.2

x	$N = \frac{1}{h}$			
	10	20	40	60
0.0	0.3161375	0.3165530	0.3166751	0.3166751
0.1	0.3128975	0.3131708	0.3132412	0.3132533
0.2	0.3026895	0.3029309	0.3029934	0.3030041
0.3	0.2857503	0.2859701	0.2860272	0.2860369
0.4	0.2622603	0.2624607	0.2625128	0.2625217
0.5	0.2324534	0.2326335	0.2326803	0.2326884
0.6	0.1966152	0.1967719	0.1968125	0.1968197
0.7	0.1550750	0.1552033	0.1552365	0.1552424
0.8	0.1081967	0.1082902	0.1083143	0.1083187
0.9	0.0563698	0.0564209	0.0564340	0.0564364

Table 6.4

Comparison Table for Problem 6.2

$(h = \frac{1}{64})$

x	Finite Difference [83]	Patch bases [83]	Our Method	Smaller Solution
0.000	0.31762	0.31672	0.3166778	0.31669
0.125	0.31135	0.31135	0.3113296	0.31134
0.250	0.29537	0.29537	0.2953528	0.29536
0.375	0.26909	0.26909	0.2690043	0.26901
0.625	0.18696	0.18696	0.1869479	0.18695
0.750	0.13243	0.13243	0.1324257	0.13243
0.875	0.069854	0.069854	0.0698503	0.069853

Smaller solution corresponds to the exact solution with

$B = 3-2\ \ 2$.

TABLE 6.5

Numerical Results for Problem 6.3

($\lambda = 0.8$)

x	h			
	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{60}$
0.0	0.2428968	0.24012132	0.2394465	0.2392885
0.1	0.2384225	0.2370623	0.2367227	0.2366591
0.2	0.2303030	0.2293343	0.2290929	0.2290477
0.3	0.2173883	0.2166573	0.2164754	0.2164412
0.4	0.1996513	0.1990947	0.1989563	0.1989302
0.5	0.1771833	0.1767655	0.1766617	0.1766421
0.6	0.1501282	0.1498253	0.1497502	0.1497360
0.7	0.1186656	0.1184597	0.1184087	0.1183990
0.8	0.0830023	0.0828782	0.0828474	0.0828416
0.9	0.0433660	0.0433102	0.0432964	0.0432938

Table 6.6

Numerical Results for Problem 6.4

$(\beta = \varphi = \gamma = 1)$

x	h = $\frac{1}{10}$	h = $\frac{1}{20}$	h = $\frac{1}{40}$	h = $\frac{1}{60}$
0.0	0.8359614	0.8365633	0.8367104	0.8367368
0.1	0.8382945	0.8383463	0.8383594	0.8383613
0.2	0.8431136	0.8431656	0.8431787	0.8431808
0.3	0.8511594	0.8512115	0.8512247	0.8512270
0.4	0.8624522	0.8625039	0.8625172	0.8625196
0.5	0.8770181	0.8770684	0.8770817	0.8770842
0.6	0.8948878	0.8949352	0.8949478	0.8949505
0.7	0.9160937	0.9161358	0.9161470	0.9161497
0.8	0.9406663	0.9406997	0.9407087	0.9407107
0.9	0.9686306	0.9686505	0.9686559	0.9686570

Table 6.7

Numerical Results for Problem 6.4

($\beta = 0.05$, $\gamma = 20$, $\varphi = 6$)

x	h = 1/10	h = 1/20	h = 1/40	h = 1/60
0.0	0.0015588	0.0017349	0.0017841	0.0018013
0.1	0.0018073	0.0020163	0.0020826	0.0020943
0.2	0.0027098	0.0030297	0.0031299	0.0031475
0.3	0.0048277	0.0053973	0.0055753	0.0056065
0.4	0.0095302	0.0106401	0.0109880	0.0110492
0.5	0.0200037	0.0222778	0.0229932	0.0231190
0.6	0.0436007	0.0483495	0.0498419	0.0501037
0.7	0.0971114	0.1068313	0.1098473	0.1103717
0.8	0.2175953	0.2356493	0.2410369	0.2419535
0.9	0.4795661	0.5039730	0.5106301	0.5117135

CHAPTER VII

IMBEDDING METHODS TO INFINITE INTERVAL PROBLEMS

7.1 Introduction.: The object of this chapter is to describe the approach of asymptotic boundary condition to solve boundary value problems on semi-infinite intervals. As discussed in Chapter 1, early attempts to treat these problems are to replace them by finite interval problems, before computing the solutions. Also one can reduce the problem to finite interval by coordinate transformation.

Following the lines of Fox [42] a second order finite difference method has been discussed by Robertson [80] for a boundary value problem on infinite interval, by truncating it to a finite interval problem. Truncation procedure has been applied by many authors. Similarly using the coordinate transformation technique, Grosch and Oraszag [46] presented a Chebyshev polynomial approach to solve some physical problems on infinite intervals. The author reduces the infinite interval problems to finite interval on $[-1,1]$ using the transformations and employed the Chebyshev polynomial approach to solve the problems. Many authors also followed the transformation procedure to solve these problems by ignoring the effect of singularity. Recently Lentini and Keller [62] have analyzed these problems by determining appropriate asymptotic

boundary conditions at a finite point. Markowich [64] has also described an adhoc method to solve boundary value problems which are posed on infinite intervals by reducing the infinite interval to a finite but large and to impose additional boundary condition at the far end.

In this chapter, we have presented an asymptotic boundary condition for the numerical solution of the point boundary value problem posed on infinite interval. By reducing the infinite interval to a finite interval which is large and imposing appropriate asymptotic boundary condition at the finite point, the resulting boundary value problem is treated by using invariant imbedding methods. The tridiagonal system resulting from imbedding is effeciently solved. The stability of the method is analysed. The transformation technique has been briefly included as an alternative method. The numerical solutions for the model problems have also been presented.

7.2 Asymptotic Boundary Condition :

We consider boundary value problems on infinite intervals in the following way :

$$Ly(x) \equiv y''(x)+f(x)y'(x)+g(x)y(x)=r(x), \quad a \leq x < \infty \qquad (7.1)$$

subject to boundary conditions

$$y(a) = \alpha \qquad (7.2)$$

$$y(\infty) = \beta \qquad (7.3)$$

$$\text{or} \quad \lim_{x\to\infty} y(x) = \beta$$

where the functions $f(x)$, $g(x)$ and $r(x)$ are continuous and $g(x) < 0$. We rewrite the Eqn. (7.1) as a first order system in the form :

Let $y(x) = u(x)$, $y'(x) = u'(x) = v(x)$, we have

$$u'(x) = v(x) \tag{7.4}$$

$$v'(x) = -f(x)\, v(x) - g(x)u(x)+r(x) \tag{7.5}$$

and correspondingly (7.2) and (7.3) become

$$u(a) = \alpha \tag{7.6}$$

$$\lim_{x\to\infty} u(x) = u_\infty = \beta \tag{7.7}$$

Letting $U = (u,v)^t$, (t denotes transpose), we can write the first order system (7.4) - (7.5) in the matrix vector form

$$U' = A(x)U + B(x) \tag{7.8}$$

$$= F(x,u) \tag{7.9}$$

where

$$A(x) = \begin{bmatrix} 0 & 1 \\ -f(x) & -g(x) \end{bmatrix}, \qquad B(x) = \begin{bmatrix} 0 \\ r(x) \end{bmatrix}$$

A general theory for linear and nonlinear systems of the form (7.8) on semi-infinite interval has been discussed by Lentini and Keller [62]. We assume that (i) $\lim_{x\to\infty} A(x) = A$, a constant matrix, (ii) $\lim_{x\to\infty} \frac{dA(x)}{dx} = 0$, (iii) $A(x)$ is piecewise continuously differentiable on (a,∞), and u_∞ is required to be the root of

$\lim_{x \to \infty} F(x,u) = 0.$ We also assume that A is assumed in the canonical form such that $A = EJE^{-1} \neq 0$ (a zero matrix) and J has the block diagonal form $J = \mathrm{diag}\,(J^+, J^0, J^-)$ where J^+ contains eigenvalues of A with positive real part, J^0 the eigenvalues of A with zero real part and J^- the eigenvalues of A with a negative real part. The main idea is to find all bounded solutions and to eliminate the contribution from the unbounded solution of the equation (7.8). The behaviour at infinity of the solution of the system (7.8) is essentially given by the eigenvalues of the matrix

$$A_{inf} = \lim_{x\to\infty} A(x) = \begin{bmatrix} 0 & 1 \\ K & L \end{bmatrix}$$

where $K = \mathrm{Lt}_{x\to\infty} - f(x)$ and $L = \lim_{x\to\infty} - g(x)$. Suppose the matrix A_∞ has the eigenvalues λ_1 and λ_2, then depending upon positive real parts of the eigenvalues Real λ_1, Real $\lambda_2 \geq 0$ we find the linearly independent solution which decay exponentially at infinity and the linearly independent solutions which are bounded as $x \to \infty$. Since we need only one condition at the far end, we expect only one eigenvalue with positive real part and say the eigenvalue is λ_1. Now corresponding to this eigenvalue we introduce the projection matrix P_M of the form $P_M = [1,0]$. (If the eigenvalue λ_2 is with positive real part, we choose $P_M = [0,1]$). Correspondingly the eigenvector to λ_1 and λ_2 be denoted by E_1 and E_2 respectively such that

$E_1 = [E_{11}, E_{21}]^t$, and $E_2 = [E_{12}, E_{22}]^t$. Then the matrix of eigenvectors of A_{inf} is,

$$E = \begin{bmatrix} E_{11} & E_{21} \\ E_{21} & E_{22} \end{bmatrix}$$

This essentially allows us to find E^{-1}, (the inverse of E), for which we know that $E^{-1} A_{inf} E = \text{diag}(\lambda_1, \lambda_2)$, we write the asymptotic boundary condition as

$$\lim_{x\to\infty} P_M E^{-1} F(x,u) = 0 \qquad (7.10)$$

Eqn. (7.10) yields the condition at x = N, where N is chosen by taking different values of x for which the computed solution approximates the actual solution.

7.3 Invariant Imbedding :

In order to solve the finite interval problem, we extend the discrete invariant imbedding technique which is described in Chapter 2. For the sake of brevity, we assume that the additional boundary condition for the Eqn. (7.1) with (7.2) is of the form

$$\alpha_o\, y(x_\infty) + \beta_o\, y'(x_\infty) = k \qquad (7.11)$$

where α_o, β_o and k are constants, $x_\infty = N$, N large but finite, with $\alpha_o\beta_o \geq 0$ and $|\alpha_o| + |\beta_o| \neq 0$. This guarantees the unique solution of the two point boundary value problems given by

Eqns. (7.1), (7.2) and (7.11) exists. (cf. Keller [55]). Discretizing Eqn. (7.1) and using central difference formulae, we get after some manipulation a finite difference system of the form

$$A_i\, y_{i+1} - B_i\, y_i + C_i\, y_{i-1} = D_i, \quad i = 1,2,\ldots,n \qquad (7.12)$$

where

$$A_i = 1 + h\, f_i/2$$

$$B_i = 2 - h^2\, g_i$$

$$C_i = 1 - h\, f_i/2$$

$$D_i = h^2\, r_i\,.$$

The corresponding boundary conditions (7.2) and (7.11) can be written in the discretized form as,

$$y_0 = \alpha \qquad (7.13)$$

$$\alpha_0\, y_n + \beta_0\, \left(\frac{y_{n+1} - y_{n-1}}{2h}\right) = k$$

or

$$2h\, \alpha_0\, y_n + \beta_0\, y_{n+1} - \beta_0\, y_{n-1} = 2hk \qquad (7.14)$$

where the value of y_{n+1} at the fictious point $x = (n+1)h$ needs to be eliminated between the Eqns. (7.12), (7.13) and (7.14). We seek a difference relation of the form

$$y_{i+1} = y_i\, W_i + S_i, \quad i = 0,1,2,\ldots,n-1 \qquad (7.15)$$

where W_i and S_i corresponds to $W(x_i)$ and $S(x_i)$ and are to be determined. Using Eqns. (7.15) and (7.12) we have

$$y_i = \frac{C_i}{(B_i - A_iW_i)} y_{i-1} + \frac{(A_iS_i - D_i)}{(B_i - A_iW_i)} \tag{7.16}$$

Also from Eqn.(7.15) we get

$$y_i = W_{i-1} y_{i-1} + S_{i-1} \tag{7.17}$$

We have from Eqns. (7.16) and (7.17) we get

$$W_{i-1} = \frac{C_i}{(B_i - A_iW_i)} \tag{7.18}$$

$$S_{i-1} = \frac{(A_iS_i - D_i)}{(B_i - A_iW_i)} \tag{7.19}$$

To solve these recurrence relation for W_i and S_i ($i = n-2, \ldots, 0$), we need to know the values of W_{n-1} and S_{n-1}. From Eqn. (7.14) we have

$$y_{n+1} = y_{n-1} + \frac{2h}{\beta_o} k - \frac{2h\alpha_o}{\beta_o} y_n \tag{7.20}$$

Writing Eqn. (7.12) at $x = n$, and eliminating y_{n+1} by using Eqn. (7.20), we get

$$y_n = \frac{(A_n+C_n)}{\left(\frac{2A_nh\alpha_o}{\beta_o} + B_n\right)} y_{n-1} + \frac{\left(\frac{2hA_nk}{\beta_o} - D_n\right)}{\left(B_n + \frac{2A_nh\alpha_o}{\beta_o}\right)} \tag{7.21}$$

Using Eqn. (7.17) at x = n and comparing with Eqn. (7.21) we have

$$W_{n-1} = \frac{(A_n + C_n)}{\left(B_n + \dfrac{2A_n h\alpha_o}{\beta_o}\right)} \tag{7.22}$$

$$S_{n-1} = \frac{\left(\dfrac{2hA_n k}{\beta_o} - D_n\right)}{\left(B_n + \dfrac{2A_n h\alpha_o}{\beta_o}\right)} \tag{7.23}$$

Starting with these values of W_{n-1} and S_{n-1}, the values of W_i and S_i $(i = n-2, n-3, \ldots, 0)$ are obtained by backward substitution using Eqns. (7.18) - (7.19). The solution y_i's $(i = 1, 2, \ldots, n)$ can then be obtained from Eqn. (7.15) by using the known values of W_i's and S_i's $(i = 0, 1, 2, \ldots, n-1)$ and the known initial value y_o.

7.4 Stability :

We will now show that the method always provides a solution and is computationally stable. We examine the recurrence relation given by Eqn. (7.18). Assuming that a small error E_i has been introduced in the calculation of W_i, we have

$$\tilde{W}_i = W_i + E_i \tag{7.24}$$

and we are actually solving

$$\tilde{W}_{i-1} = \frac{C_i}{(B_i - A_i \tilde{W}_i)} \tag{7.25}$$

From Eqns. (7.25) and (7.24) we get

$$E_{i-1} \simeq W_{i-1} \frac{A_i}{C_i} W_{i-1} E_i \tag{7.26}$$

under the assumption that initially the error is small. To show $|E_{i-1}| < |E_i|$, we first show that $0 < W_i < 1$, for $i = n-1,\ldots,0$. Assume that $A_i > 0$ and $C_i > 0$ for all i and from the definition of A_i, B_i and C_i, we also have $B_i > 0$ and $B_i > C_i+A_i$.

Now

$$W_{n-1} = \frac{(A_n+C_n)}{\left(\frac{2A_n h\alpha_o}{\beta_o} + \beta_n\right)},$$

we see that under the above mentioned conditions $0 < W_{n-1} < 1$. Also

$$\begin{aligned} W_{n-2} &= \frac{C_{n-1}}{(B_{n-1} - A_{n-1} W_{n-1})} \\ &< \frac{C_{n-1}}{(B_{n-1} - A_{n-1})} \\ &< 1 \end{aligned}$$

and thus $0 < W_{n-2} < 1$. Similarly, it can recursively shown that $0 < W_i < 1$, $i = n-3,\ldots,0$. Thus the error Eqn. (7.26) gives $|E_{i-1}| < |E_i|$, provided $A_i \leq C_i$ and therefore the recurrence relation (7.22) is computationally stable. Following a similar arguments it can be shown that Eqn. (7.23) is also stable.

7.5 Coordinate Transformation :

In order to demonstrate the transformation procedure over infinite interval, we have considered different transformations for the assumed Eqn. (7.1) - (7.3). A standard procedure is let $X = a/x$, if $a \neq 0$ or $X = \frac{1}{(x+1)}$ if $a = 0$. By using algebraic transformation one may reduce Eqn. (7.1) as follows :

$$X = \frac{1}{(x+1)} \tag{7.27}$$

$$\frac{dX}{dx} = \frac{-1}{(x+1)^2} = -X^2$$

$$\frac{dy}{dx} = -X^2 \frac{dy}{dX} \tag{7.28}$$

$$\frac{d^2y}{dx^2} = X^4 \frac{d^2y}{dX^2} + 2X^3 \frac{dy}{dX} \tag{7.29}$$

By using Eqns. (7.28) - (7.29), Eqn. (7.1) becomes

$$\frac{d^2y}{dX^2} + \frac{dy}{dX} \{\frac{2}{X} - \frac{f(X)}{X^2}\} + \frac{g(X)}{X^4} y(X) = \frac{r(X)}{X^4} \tag{7.30}$$

where $f(X) = f(x)$, $g(X) = g(x)$ and $r(X) = r(x)$ with $x = \frac{(1-X)}{X}$.
The corresponding boundary conditions Eqns. (7.2) and (7.3) becomes

$$y(X) = \alpha \tag{7.31}$$

$$y(0) = \beta \tag{7.32}$$

where X is defined in Eqn. (7.27).

Similarly using an exponential transformation one may reduce the infinite interval problems to finite interval problems.

Using $X = 1-e^{-x}$, Eqn. (7.1) reduces to

$$\frac{d^2y}{dX^2} + \frac{dy}{dX}\left\{\frac{f(X)}{1-X} - \frac{1}{1-X}\right\} + \frac{g(X)}{(1-X)^2}\, y(X) = \frac{r(X)}{(1-X)} \tag{7.33}$$

with

$$y(X) = \alpha \tag{7.34}$$

$$y(1) = \beta \tag{7.35}$$

Eqns. (7.33) - (7.35) and Eqns. (7.30) - (7.32) constitutes a singular two point boundary value problem either with a regular singular point or singularity of the second kind. If one is led to the regular singular problem, then the methods discussed in Chapters 2-3 can be applied directly, by using the expansion procedure about the singular point. If the transformed problem has singularity of the second kind, one may apply a different procedure (cf. de Hoog and Weiss [32]). However, in general, these types of transformations produce a singularity of the second kind for infinite interval problems. Depending upon the physical situation one may choose a proper algebraic or exponential transformation . An obvious advantage of the change of variable approach is that no experimental choice of a large number to represent the point at infinity is necessary. This particular procedure has been applied to the problem 7.1 and the results are tabulated in Table 7.4.

7.6 Numerical examples and Discussion :

In this section some numerical examples of the model problems are solved to show the efficiency of the method.

Problem 7.1 : To illustrate our method, we solve

$$Ly \equiv -y'' - 2y' + 2y = e^{-2x}, \qquad 0 \leq x < \infty$$

subject to boundary conditions

$$y(0) = 1.0$$

$$y(\infty) = 0.0$$

This problem has earlier been solved by Robertson [80] and its exact solution is given by $y(x) = \frac{1}{2} e^{-(1+\sqrt{3})x} + \frac{1}{2} e^{-2x}$. The asymptotic boundary condition for this problem by our method is given by $2y(x_\infty) - \sqrt{3}\, y'(x_\infty) = 0$.

Problem 7.2 : As a last experiment, we solve

$$-y'' + (1 + \tfrac{1}{x})y = \frac{1}{x^2}, \qquad 1 \leq x < \infty$$

with boundary conditions

$$y(1) = 0$$

$$y(\infty) = 0.$$

Fox [42] and Robertson [80] have earlier solved this model problem. The asymptotic boundary condition for this problem by our method is given by $0.5\, y(x_\infty) + 0.5\, y'(x_\infty) = 0$.

The numerical results for problem 7.1 for different values of N are presented in Table 7.1. The values of N taken for computation are 8, 9 and 10. We observe from this table that the computed solutions compare well with the exact solution. Also the solutions are seen to compare well upto five to six decimal places of accuracy with Robertson's [80] solution at $x_\infty = 9$. The errors present in the numerical solution for these values of N are given in Table 7.2. It can be observed from results that $x_\infty = N = 9$ can be taken to represent the point at infinity for this problem.

The numerical results for Problem 7.2 are shown in Table 7.3 considering the variations in the computed solutions at different x for different step sizes, we observe that the value of $x_\infty = N$ gets smaller for smaller values of h. It is evident from the table that the solutions decay relatively slowly which agrees with the observation made by Fox [42]. The computed solutions also compare well with that obtained by Robertson [80] at $x_\infty = N = 9$. From the computational results, it thus can be stated that N = 9 represents the point at infinity for this problem.

In Table 7.4 we present the numerical solutions for the Problem 7.1 using the coordinate transformation. We applied the exponential transformation to get the finite interval problem and used the expansion procedure near to singularity which is discussed in Chapter 3. The value of $X = \delta$ as used in

Chapter 3, has been taken near the singularity (viz. $\delta = 0.9$) to observe the variation in the solutions by transformation. The computed solutions compare well with the exact solution up to five places of decimal. Though the latter method reduces the infinite interval problem to a problem on a finite interval thereby evading the computation on a larger interval (as in the former case) but the main disadvantage is that it leads, in general, to a singular problem with an essential singularity. In view of this, the technique of coordinate transformations is not practical in many cases.

TABLE 7.1

Numerical Results for Problem 7.1

$X_\infty = N$	X	h: 1/32	h: 1/64	h: 1/128	Exact Solution
8	1.0	0.1001679 E+00	0.1002006 E+00	0.1002094 E+00	0.10021047 E+00
	2.0	0.1126875 E-01	0.1127424 E-01	0.1127572 E-01	0.11275891 E-01
	3.0	0.1376269 E-02	0.1377013 E-02	0.1377214 E-02	0.1377232 E-02
	5.0	0.2328492 E-04	0.2329708 E-04	0.2330009 E-04	0.2328394 E-04
	7.0	0.4921775 E-06	0.4923843 E-06	0.4924277 E-06	0.4182382 E-06
	8.0	0.2107120 E-06	0.2107436 E-06	0.2107493 E-06	0.56428597 E-07
9	2.0	0.1126874 E-01	0.1127424 E-01	0.1127572 E-01	0.1127589 E-01
	4.0	0.1765793 E-03	0.1766756 E-03	0.1767016 E-03	0.17670377 E-03
	5.0	0.2326888 E-04	0.2328126 E-04	0.2328461 E-04	0.2328394 E-04
	6.0	0.3110317 E-05	0.3111907 E-05	0.3112300 E-05	0.3110115 E-05
	8.0	0.6641547 E-07	0.6644302 E-07	0.6644880 E-07	0.56428597 E-07
	9.0	0.2846338 E-07	0.2846755 E-07	0.2846831 E-07	0.76254693 E-08
10	2.0	0.1126874 E-01	0.1127424 E-01	0.1127572 E-01	0.1127589 E-01
	4.0	0.1765788 E-03	0.1766751 E-03	0.1767012 E-03	0.17670377 E-03
	6.0	0.3108151 E-05	0.3109769 E-05	0.3110208 E-05	0.3110115 E-05
	7.0	0.4182718 E-06	0.4182819 E-06	0.4185339 E-06	0.4182382 E-06
	9.0	0.8975769 E-08	0.8979465 E-08	0.8980238 E-08	0.76254693 E-08
	10.0	0.3848627 E-08	0.3849183 E-08	0.3849284 E-08	0.103125887 E-08

TABLE 7.2

Errors in the numerical solution for Problem 7.1
for different values of N

$X_{\infty} = N$	X	h: 1/64	h: 1/128
8	2.0	0.165 E-05	0.171 E-06
	4.0	0.293 E-07	0.325 E-08
	6.0	0.323 E-08	0.279 E-08
	8.0	0.119 E-07	0.119 E-08
9	2.0	0.165 E-05	0.171 E-06
	4.0	0.287 E-07	0.264 E-09
	6.0	0.661 E-09	0.219 E-09
	8.0	0.782 E-09	0.774 E-09
	9.0	0.161 E-09	0.161 E-09

TABLE 7.3

Numerical Results for Problem 7.2

x	h = 1.0	h = 0.5	h = 0.25	h = 0.125
1.0	0.0000000 E+0	0.0000000 E+0	0.0000000 E+0	0.0000000 E+0
5.0	0.4035932 E-01	0.3985671 E-01	0.3914139 E-01	0.3910466 E-01
7.0	0.2132566 E-01	0.2005994 E-01	0.2005561 E-01	0.2005166 E-01
9.0	0.1194996 E-01	0.1195345 E-01	0.1195671 E-01	0.1195712 E-01
25.0	0.1550507 E-02	0.1551536 E-02	0.1552544 E-02	0.1550714 E-02
30.0	0.1082105 E-02	0.1081996 E-02	0.1082996 E-02	-
31.0	0.1013287 E-02	0.1013988 E-02	-	-
45.0	0.1013998 E-02	0.4843556 E-03	-	-
55.0	0.4843976 E-03	-	-	-
65.0	0.3056754 E-03	-	-	-

TABLE 7.4

Numerical results for Problem 7.1
using Transformation

X	δ					
	0.4	0.5	0.6	0.7	0.9	Exact Solution
0.0	1.000000	1.000000	1.000000	1.000000	1.000000	1.0000000
0.1	0.7799359	0.7799350	0.7799380	0.7799456	0.7800392	0.7799369
0.2	0.5917713	0.5917696	0.5917757	0.5917899	0.5919696	0.5917734
0.3	0.4336952	0.4336927	0.4337010	0.4337237	0.4339833	0.4336992
0.4	0.3038358	0.3038325	0.3038435	0.3038713	0.3042130	0.3038420
0.5	–	0.2002429	0.2002566	0.2002914	0.2007194	0.2002559
0.6	–	–	0.1208999	0.1209431	0.1214742	0.1209051
0.7	–	–	–	0.0636504	0.0643239	0.0636969
0.8	–	–	–	–	0.0269258	0.02615670
0.9	–	–	–	–	0.00614024	0.0059267

CHAPTER VIII

Cubic Spline Solutions of Boundary Value Problems over Infinite Interval

8.1 Introduction : The development of improved methods for solving two point boundary value problems of practical significance is of great important in Science and Engineering. In many cases the domain of the governing equations of these problems is infinite or semi-infinite so that the special treatment is required to these so called infinite interval problems. These problems occur very frequently and are of great importance in areas such as fluid dynamics, aerodynamics etcetera. Often in most cases the analytical solutions for these problems are not readily attainable and thus the problem is brought to the problem of finding efficient computational algorithms for obtaining the numerical solution.

Ever since the pioneering work by Ahlberg et al. [2] there has been a great deal of development in the theory of spline functions and their applications to several practical problems. Of these, the cubic splines have attained a prime place and have attracted the attention of many to solve, in particular, boundary value problems. This is possibly because these cubic splines are efficient and simple to use and possess important properties that are required of a good approximation. To cite a few, Bickley [14] has considered the use of cubic

spline for solving linear two point boundary value problems, which leads to the solution of a set of linear equations whose coefficients matrix is of upper Hessenberg form. The cubic spline method suggested by Bickley has also been examined by Fyfe [45] in combination with deferred correction to solve two point boundary value problems. The cubic spline approximation has been applied by **Albasiny** and Hoskins [4] to an integral equation reformulation of the original differential equation, which have been shown to have smaller truncation error than would be obtained by direct use of the cubic spline on the differential equation itself. In another paper by the same authors [3], the spline solutions have been obtained by solving a set of equation with a tridiagonal matrix of coefficients. Daniel [28] has proposed the use of acceleration with collocation with various types of spline approximation appropriate for two point boundary value problems. There are several other papers on this topic, but little seems to have been done in using cubic splines to solve boundary value problems over infinite intervals.

In this chapter we present a cubic spline procedure for numerically solving boundary value problems over infinite intervals. Unlike the familiar three point finite difference scheme second order accuracy is maintained even with a non-uniform mesh and relatively large changes in the grid spacing. Also spline approximations described here leads to tridiagonal systems. The asymptotic boundary condition for the infinite

interval problems is derived. The cubic spline formulation and the procedure is discussed with derivative boundary conditions. The tridiagonal system has been solved efficiently and the stability of the method is discussed. Numerical examples for the model problems are given.

8.2 Asymptotic Boundary Condition :

We consider the linear two point boundary value problems of the form

$$Ly(x) \equiv y''(x)+P(x)y'(x)+Q(x)y(x) = R(x), \; a \leq x < \infty \qquad (8.1)$$

subject to boundary conditions

$$\left.\begin{aligned} y(a) &= \alpha \\ y(\infty) &= \beta \end{aligned}\right\} \qquad (8.2)$$

$$\text{or} \qquad \lim_{x\to\infty} y(x) = \beta \qquad (8.3)$$

where the function $P(x)$, $Q(x)$ and $R(x)$ are continuous and $Q(x) < 0$. In order to find the appropriate boundary conditions for the Eqn. (8.1) we rewrite (8.1) as a first order system in the form

$$u'(x) = v(x) \qquad (8.4)$$

$$v'(x) = -P(x)v(x)-Q(x)u(x)+R(x) \qquad (8.5)$$

where $y(x) = u(x)$, $y'(x) = u'(x) = v(x)$. Correspondingly (8.2) – (8.3) became

$$u'(a) = \alpha \tag{8.6}$$

$$\underset{x\to\infty}{\mathrm{Lt}}\ u(x) = \beta \tag{8.7}$$

Letting $U = (u,v)^t$, (t denotes transpose), we can write the first order system (8.4) - (8.5) in the matrix vector form

$$\begin{aligned} U' &= A(x)U + f(x) \qquad (8.8) \\ &= F(x,U) \end{aligned}$$

where

$$A(x) = \begin{bmatrix} 0 & 1 \\ -Q(x) & -P(x) \end{bmatrix}, \quad f(x) = \begin{bmatrix} 0 \\ R(x) \end{bmatrix}$$

As discussed in the earlier chapter, the method requires that the matrix $A(x)$ should be a constant matrix as $x \to \infty$. Also the main idea is to eliminate contributions from the unbounded solution of the equation, which are essentially given by the eigenvalues of the matrix $A(x)$. Let A_{inf} denote the matrix when $x \to \infty$ so that

$$A_{inf} = \underset{x\to\infty}{\mathrm{Lt}}\ A(x) = \begin{bmatrix} 0 & 1 \\ K & L \end{bmatrix}$$

where $K = \underset{x\to\infty}{\mathrm{Lt}} - Q(x)$ and $L = \underset{x\to\infty}{\mathrm{Lt}} - P(x)$. Suppose the matrix A_{inf} has the eigenvalues λ_1 and λ_2, then depending upon Real λ_1, Real $\lambda_2 \geq 0$, one can find linearly independent solutions at infinity and the corresponding projection matrix. Let E be the matrix of eigenvectors of A_{inf}, then by calculating E^{-1} for which

$E^{-1} A_{inf} E = \text{diag}(\lambda_1, \lambda_2)$, we write the asymptotic condition as

$$\lim_{x \to \infty} P_M E^{-1} F(x, U) = 0 \tag{8.9}$$

Eqn. (8.9) yields the condition at $x = N$ where N is chosen by taking different values of x for which the computed solution approximates the actual solution.

8.3 Cubic Spline Formulation :

We now describe a cubic spline procedure to solve the finite interval problem obtained by asymptotic boundary condition. For the sake of brevity, we assume that the Eqn. (8.9) is of the form

$$\alpha_o\, y(x_\infty) + \beta_o\, y'(x_\infty) = K \tag{8.10}$$

for $x_\infty = N$, N large but finite, where α_o, β_o and K are known constants such that $\alpha_o \beta_o \geq 0$ and $|\alpha_o| + |\beta_o| \neq 0$. This guarantees the unique solution of the two point boundary value problem given by Eqns. (8.1), (8.2) and (8.10) (cf. Keller [55]).

We consider a mesh with grid points $a = x_o < x_1 < x_2 \cdots < x_n = N$ with $h = x_i - x_{i-1} > 0$. The function $y(x)$ at the node points x_i is denoted by $y(x_i) = y_i$. Let $S_p(y;x) = S_p(x)$ denote the cubic spline function, which is continuous together with its first and second derivatives on $[a, N]$ and satisfies $S_p(x_i) = y_i$. Then in general :

$$S_p''(x) = M_{i-1} \frac{(x_i - x)}{h} + M_i \frac{(x - x_{i-1})}{h} \tag{8.11}$$

where $M_i = S_p''(x_i)$.

Integrating Eqn. (8.11) twice results in the spline interpolation formula on (x_i, x_{i-1}) :

$$S_p(x) = M_{i-1}\frac{(x_i-x)^3}{6h} + M_i\frac{(x-x_{i-1})^3}{6h} + (y_{i-1} - \frac{M_{i-1}h^2}{6})\frac{(x_i-x)}{h}$$

$$+ (y_i - \frac{M_i h^2}{6})\frac{(x_i-x_{i-1})}{h} \qquad (8.12)$$

where the integration constants have been evaluated by the requirement of continuity of the spline function and its first derivative at the node points. Ahlberg et al. [2] have shown that if the function $y(x) \varepsilon C^4 [a,N]$, then the spline function $S_p(x)$ approximates $y(x)$ at all points in $[a,N]$ to fourth order in h. The unknown derivatives M_i are related by enforcing the continuity condition on $S_p'(x)$.

Differentiating (8.12), we get

$$S_p'(x) = M_{i-1}\left[-\frac{(x_i-x)^2}{2h} + \frac{h}{6}\right] + M_i\left[\frac{(x-x_{i-1})^2}{2h} - \frac{h}{6}\right] + \frac{(y_i-y_{i-1})}{h} \qquad (8.13)$$

From Eqn. (8.13) we have the one sided limits of the derivatives as

$$S_p'(x+) = \frac{(y_{i+1}-y_i)}{h} - \frac{h}{3}M_i - \frac{h}{6}M_{i+1}, \quad i = 0,1,2,\ldots,n-1 \qquad (8.14)$$

and

$$S_p'(x-) = \frac{(y_i-y_{i-1})}{h} + \frac{h}{3}M_i + \frac{h}{3}M_{i-1}, \quad i = 1,2,\ldots,n \qquad (8.15)$$

By virtue of (8.11) and (8.12) the functions $S_p''(x)$ and $S_p(x)$ are continuous on $[a,N]$, the continuity of $S_p'(x)$ at x_i yields by means of Eqns. (8.14) - (8.15) the condition as

$$\frac{h}{6} M_{i-1} + \frac{2h}{3} M_i + \frac{h}{6} M_{i+1} = \frac{y_{i+1}-y_i}{h} - \frac{(y_i-y_{i-1})}{h} \qquad i = 1,2,\ldots,n-1 \tag{8.16}$$

Employing spline approximation (8.13) to the Eqn. (8.1) and using (8.14) - (8.15), we have for $i = 0,1,2,\ldots,n-1$,

$$M_i + P_i \left[\frac{y_{i+1}-y_i}{h} - \frac{h}{3} M_i - \frac{h}{6} M_{i+1}\right] + Q_i y_i = R_i$$

or

$$(1-\frac{h}{3}P_i)M_i - \frac{h}{6} P_i M_{i+1} + \frac{P_i}{h} (y_{i+1}-y_i)+Q_i y_i = R_i \tag{8.17}$$

and similarly for $i = 1,2,\ldots,n$,

$$(1 + \frac{h}{3}P_i)M_i + \frac{h}{6} P_i M_{i-1} + \frac{P_i}{h} (y_i-y_{i-1})+Q_i y_i = R_i \tag{8.18}$$

Also from Eqns. (8.17) and (8.18), we get a relationship

$$2M_i + \frac{h}{6} P_i M_{i-1} - \frac{h}{6} P_i M_{i+1} + \frac{P_i}{h} (y_{i+1}-y_{i-1}) = 2R_i-2Q_i y_i$$

$$i = 1,2,\ldots,n-1. \tag{8.19}$$

To find the cubic polynomial $S_p(x)$ at different points we need the unknown coefficients M_{i-1}, M_i and M_{i+1} in the Eqn. (8.12). We eliminate M_i's $(i = 0,1,\ldots,n)$ from Eqns. (8.17) and (8.18). From Eqn. (8.17), we replace i by $i-1$ and get

$$(1-\frac{h}{3}P_{i-1})M_{i-1}-\frac{h}{6}P_{i-1}M_i+\frac{P_{i-1}}{h}(y_i-y_{i-1})+Q_{i-1}y_{i-1}=R_{i-1} \tag{8.20}$$

From Eqns. (8.20) and (8.18) by eliminating M_i we have,

$$M_{i-1}=\frac{1}{a_i}[(P_{i-1}+\frac{h}{3}P_iR_{i-1}+\frac{h}{6}P_{i-1}R_i)$$
$$-y_{i-1}(Q_{i-1}+\frac{h}{3}P_iQ_{i-1}-\frac{P_{i-1}}{h}-\frac{P_iP_{i-1}}{2})$$
$$-y_i(\frac{P_{i-1}}{h}+\frac{h}{6}P_{i-1}Q_i+\frac{P_iP_{i-1}}{2})],i=1,2,\ldots,n \tag{8.21}$$

$$\text{where } a_i=1-\frac{h}{3}P_{i-1}+\frac{h}{3}P_i-\frac{h^2}{12}P_iP_{i-1} \tag{8.22}$$

Again from Eqn. (8.17), we replace i by (i+1) and get,

$$M_{i+1}=\frac{1}{b_i}[(P_{i+1}-\frac{h}{3}P_iR_{i+1}-\frac{h}{6}P_{i+1}R_i)$$
$$-y_{i+1}(Q_{i+1}-\frac{h}{3}P_i\,R_{i+1}+\frac{P_{i+1}}{h}-\frac{P_iP_{i+1}}{2})$$
$$+y_i(\frac{P_{i+1}}{h}-\frac{P_iP_{i+1}}{2}+\frac{h}{6}P_{i+1}Q_i)]\;,i=0,1,2,\ldots,n-1 \tag{8.23}$$

$$\text{with}\quad b_i=1-\frac{h}{3}P_i+\frac{h}{3}P_{i+1}-\frac{h^2}{12}P_iP_{i+1} \tag{8.24}$$

By substracting Eqn. (8.16) from Eqn. (8.19) we get an expression as

$$y_{i-1}(1 - \frac{h}{3} P_i) - y_i(2 - \frac{2h^2}{3} Q_i) + y_{i+1}(1 + \frac{h}{3} P_i)$$

$$= \frac{2h^2}{3} R_i + \frac{h^2}{6} (1 - \frac{h}{3}P_i)M_{i-1} + \frac{h^2}{6} (1 + \frac{h}{3}P_i)M_{i+1} \qquad (8.25)$$

$$i = 1, 2, \ldots, n-1.$$

Using Eqns. (8.21) and (8.23) in (8.25), we have after some algebric manipulation a tridoagonal system given by

$$D_i\, y_{i-1} - C_i y_i + E_i\, y_{i+1} = F_i,\ i = 1, 2, \ldots, n-1 \qquad (8.26)$$

where D_i, C_i, E_i and F_i are given by the equations

$$D_i = b_i \left[1 - \frac{h}{2} P_{i-1} + \frac{h^2}{6} Q_{i-1})\right] \qquad (8.27)$$

$$C_i = \left[a_i(1 + \frac{h}{2} P_{i+1}) + b_i(1 - \frac{h}{2} P_{i-1})\right.$$

$$\left. - \frac{2h^2}{3} Q_i(1 - \frac{h^2}{12} P_{i-1}P_{i+1} + \frac{7h}{24} (P_{i+1} - P_{i-1})\right] \qquad (8.28)$$

$$E_i = a_i \left[1 + \frac{h}{2} P_{i+1} + \frac{h^2}{6} Q_{i+1}\right] \qquad (8.29)$$

and

$$F_i = \frac{1}{6} \left[h^2 b_i R_{i-1} + 4h^2 R_i(1 - \frac{h^2}{12} P_{i-1}P_{i+1} + \frac{7h}{24} (P_{i+1} - P_{i-1}))\right.$$

$$\left. + h^2 a_i R_{i+1}\right]. \qquad (8.30)$$

8.4 Computational Method :

To solve the tridiagonal system given by (8.26) we seek a difference relation of the form

$$y_{i+1} = W_i y_i + T_i, \quad i = 0, 1, 2, \ldots, n-1 \tag{8.31}$$

where W_i and T_i correspond to $W(x_i)$ and $T(x_i)$ and are to be determined. By using (8.31) in (8.26), we have

$$y_i = \frac{D_i}{(C_i - E_i W_i)} y_{i-1} + \frac{(E_i T_i - F_i)}{(C_i - E_i W_i)} \tag{8.32}$$

But from (8.31), we have

$$y_i = W_{i-1} y_{i-1} + T_{i-1}. \tag{8.33}$$

From Eqns. (8.32) and (8.33), we get

$$W_{i-1} = \frac{D_i}{(C_i - E_i W_i)} \tag{8.34}$$

and

$$T_{i-1} = \frac{(E_i T_i - F_i)}{(C_i - E_i W_i)} \tag{8.35}$$

To solve the recurrence relation for W_i and T_i $(i = n-2, \ldots, 0)$ we need to know the values of W_{n-1} and T_{n-1}.

From Eqn. (8.10) for $x = n$, we have

$$\alpha_0 y_n + \beta_0 y'_n = K \tag{8.36}$$

Eqn. (8.36) can be approximated at $x = n$ by using the expressions (8.15), (8.21) and (8.23), we have

$$\alpha_1 y_n - \beta_1 y_{n-1} = \gamma_1 \tag{8.37}$$

a two term relationship in y_{n-1} and y_n, where

$$\alpha_1 = \alpha_o + \frac{h}{3a_n} \beta_o(-Q_n - \frac{P_n}{h} - \frac{P_{n-1}}{2h} + \frac{h}{4} P_{n-1} Q_n + \frac{P_n P_{n-1}}{4} + \frac{3a_n}{h^2}) \tag{8.38}$$

$$\beta_1 = \frac{h}{3a_n} \beta_o(-\frac{P_n}{h} - \frac{P_{n-1}}{2h} + \frac{Q_{n-1}}{2} + \frac{P_n P_{n-1}}{4} + \frac{3a_n}{h^2}) \tag{8.39}$$

and

$$\gamma_1 = K + \frac{h}{3a_n} \beta_o(-R_n \frac{R_{n-1}}{2} + \frac{h}{4} P_{n-1} R_n) \tag{8.40}$$

From (8.33) for $i = n$ we have

$$y_n = W_{n-1}\, y_{n-1} + T_{n-1} \tag{8.41}$$

Comparing (8.37) and (8.41), we obtain W_{n-1} and T_{n-1} as

$$W_{n-1} = \beta_1/\alpha_1 \tag{8.42}$$

$$T_{n-1} = \gamma_1/\alpha_1 \tag{8.43}$$

Then W_i's and T_i's $(i = n-2, n-3, \ldots, 0)$ are obtained recursively in the backward process by using Eqns. (8.34) – (8.35). Using the values of W_i's and T_i's and knowing the value of y_o, the solution y_i's $(i = 0, 1, \ldots, n)$ can be obtained by forward process by using (8.31).

8.5 Stability : We now examine the recurrence relation given by Eqns. (8.34) – (8.35) for stability. Assume that a small error ε_i has been introduced in the calculation of W_i then we have

$$\tilde{W}_i = W_i + \varepsilon_i \tag{8.44}$$

and we are actually solving

$$\tilde{W}_{i-1} = -\frac{D_i}{(C_i - E_i \tilde{W}_i)} \tag{8.45}$$

From Eqns. (8.34) and (8.45), we have

$$\varepsilon_{i-1} = W_{i-1} \frac{E_i}{D_i} \varepsilon_i W_{i-1} , \tag{8.46}$$

under the assumption that initially the error is small.

Let us assume that $E_i > 0$ and $D_i > 0$ for $1 \leq i \leq n-1$, then from the definition of D_i, C_i, E_i and since $Q(x) < 0$, it can be easily verified that $C_i > D_i+E_i$ for $1 \leq i \leq n-1$. From Eqn. (8.42), we have $W_{n-1} = \beta_1/\alpha_1$, and $|W_{n-1}| < 1$, if $M > 0$ and $\beta_1 > -M/2$, where $M = \alpha_o + \frac{h}{3a_n} \beta_o \left(-Q_n - \frac{Q_{n-1}}{2} + \frac{h}{4} P_{n-1} Q_n\right)$. Under this condition and making use of the assumptions on D_i, C_i and E_i, it follows very easily from (8.34) that

$$|W_i| < 1, \text{ for } i = n-2, n-3, \ldots, 0 \tag{8.47}$$

and thus $|W_i| < 1$, $i = 0,1,2,\ldots,n-1$. From Eqn. (8.46), it then follows that

$$|\varepsilon_{i-1}| = |W_{i-1}|^2 \frac{|E_i|}{|D_i|} |\varepsilon_i|$$

$$< |\varepsilon_i|, \text{ provided } |E_i| \leq |D_i|$$

making the recurrence relation (8.34) stable. Similar arguments will show that the recurrence relation (8.35) is also stable.

8.6 Numerical examples and Discussion :

In this section, the numerical results of the two model problems solved are given to illustrate the method and its effectiveness.

Problem 8.1 : We solve

$$Ly(x) \equiv -y'' - 2y' + 2y = e^{-2x}, \qquad 0 \leq x < \infty,$$

with boundary conditions

$$y(0) = 1$$

$$\operatorname*{Lt}_{x\to\infty} y(x) = 0.$$

This problem has earlier been solved by Robertson [80] and its exact solution is given by $y(x) = \frac{1}{2}\, e^{-(1+\sqrt{3})x} + \frac{1}{2}\, e^{-2x}$. The asymptotic condition obtained by our method for this example is given by

$$\frac{1}{\sqrt{3}}\, y(x_\infty) + \frac{1}{2\sqrt{3}}\,(-1 + \sqrt{3})\,y'(x_\infty) = 0.$$

Problem 8.2 : As a second example, we solve

$$Ly(x) \equiv -y'' + (1 + \tfrac{1}{x})y = \frac{1}{x^2}, \qquad 1 \leq x < \infty$$

subject to boundary conditions

$$y(1) = 0$$

$$\lim_{x\to\infty} y(x) = 0.$$

This problem has earlier been considered by Fox [42] and later by Robertson [80]. The asymptotic boundary condition is given by $\frac{1}{2}\, y(x_\infty) + \frac{1}{2}\, y'(x_\infty) = 0.$

Table 8.1 represents numerical solutions for Problem 8.1 at some selected points by taking different mesh size h and different values of $x_\infty = N$. The values of N taken for computation are N = 10, 11 and 12. The exact solution of the problem is also presented and it is observed that the computed solutions compare favourably well with the exact solution. It is known for this example that the solution decays exponentially and this fact is reflected in the computed solutions for different values of N. It can be seen that the computed solutions for N = 12 give atleast six place occuracy and thus N = 12 can be taken to represent the point at infinity for this problem.

The numerical solutions for Problem 8.2 for different values of h are given in Table 8.2. It is observed from this table that the solutions decay relatively slowly which agrees with the observation made by Fox [42]. The computed solutions also compare very well with that obtained by Robertson [80] and at $x_\infty = N = 9$, the solution compare upto five places of decimal. The advantage of using cubic spline is that it not only gives an approximation to the solution y(x) but also an approximation to the derivative y'(x) at every point of the interval.

TABLE 8.1

Numerical Solution for Problem 8.1

$x_\infty=N$	x	h: 1/32	1/64	1/128	Exact Solution
10	3.0	0.13759746 E-02	0.137691756 E-02	0.13771534 E-02	0.13772232 E-02
	6.0	0.31078798 E-05	0.31095814 E-05	0.31100070 E-05	0.31101148 E-05
	8.0	0.56548516 E-07	0.56572160 E-07	0.56576829 E-07	0.56428597 E-07
	10.0	0.17141544 E-08	0.16931479 E-08	0.16824897 E-08	0.10312569 E-08
11	3.0	0.13759746 E-02	0.13769176 E-02	0.137715343E-02	0.13772321 E-02
	6.0	0.31078456 E-05	0.31095483 E-05	0.31099744 E-05	0.31101148 E-05
	8.0	0.56400702 E-07	0.56428997 E-07	0.56435997 E-07	0.56428597 E-07
	10.0	0.10750475 E-08	0.10741567 E-08	0.10735823 E-08	0.10312569 E-08
	11.0	0.23189027 E-09	0.22904771 E-09	0.22760567 E-09	0.13951780 E-09
12	3.0	0.13759746 E-02	0.13769176 E-02	0.13771535 E-02	0.13772321 E-02
	6.0	0.31078433 E-05	0.31095461 E-05	0.31099723 E-05	0.31101148 E-05
	8.0	0.56391087 E-07	0.56419684 E-07	0.56426836 E-07	0.56428597 E-07
	10.0	0.10334734 E-08	0.10338912 E-08	0.10339729 E-08	0.10312569 E-08
	12.0	0.31376740 E-10	0.30992060 E-10	0.30796922 E-10	0.18878562 E-10

TABLE 8.2

Numerical Solution for Problem 8.2

X	h				
	1.0	0.5	0.25	0.125	0.0625
1.0	0.000000	0.000000	0.000000	0.000000	0.000000
5.0	0.403603 E-01	0.393816 E-01	0.391047 E-01	0.391046 E-01	0.390915 E-01
7.0	0.201316 E-01	0.200668 E-01	0.200455 E-01	0.200454 E-01	0.200445 E-01
9.0	0.119507 E-01	0.119559 E-01	0.119570 E-01	0.119570 E-01	0.119571 E-01
15.0	0.427250 E-02	0.427326 E-02	0.427345 E-02	0.427350 E-02	0.427350 E-02
25.0	0.1552507E-02	0.155254 E-02	0.155254 E-02	0.155072 E-02	-
30.0	0.108212 E-02	0.108213 E-02	0.108203 E-02	-	-
31.0	0.101408 E-02	0.101409 E-02	0.101409 E-02	-	-
45.0	0.484474 E-03	0.484474 E-03	0.468083 E-03	-	-
55.0	0.325300 E-03	0.325306 E-03	-	-	-
65.0	0.233423 E-03	-	-	-	-
75.0	0.173966 E-03	-	-	-	-
77.0	0.153022 E-03	-	-	-	-

<u>BIBLOGRAPHY</u>

[1] Ahlberg, J.H. : A collocation method for two point boundary value problems, Math.Comp., 29(1975), 761-776.

[2] Ahlberg, J.H., Nilson, E. and Walsh, J.L. : The theory of splines and their applications, Academic Press, New York, 1967.

[3] **Albasiny**, E.L. and: Hoskins, W.D. Cubic spline solution to the two point boundary value problems, Comp.J., 12(1969), 151-153.

[4] ______ : Increased accuracy cubic splines to two point boundary value problems. J.Inst. Maths and Applic 9(1972), 47-55.

[5] Alspaugh, D.W. : The application of invariant imbedding to the solution of linear two point boundary value problems on an infinite interval, Math.Comp., 28(1974), 1005-1015.

[6] Alspaugh, D.W. Kagiwada, H.W. and Kalaba, R. : Application of invariant imbedding to the backing columns, J.C. P., 5(1970), 56-69.

[7] Angel, E. and Bellman, R. : Dynamic programming and partial differential equations, Academic Press, New York, 1972.

[8] Ascher, U. and Russell, R.D. : Reformulation of boundary value problems into standard form, SIAM Review, 23(1983), 238-254.

[9] Bailey, P.B. and Wing, G.M. : Some recent developments in invariant imbedding with applications, J. Math.Phy., 6(1965), 453-462.

[10] Banks, D.O. and Kurowski, G.J. : Computation of eigenvalues of Singular sturm-**Liouville** systems, Math.Comp, 22(1968), 304-310.

[11] Bellman, R., Kagiwada, H.H. and Kalaba, R. : Invariant imbedding and the numerical integration of boundary value problems for unstable linear systems of ordinary differential equations, Communs. ACM., 2(1967), 100-102.

[12] Bellman, R. and Kalaba, R. : Quasilinearization and Nonlinear boundary value problems, Elsevier, New York, 1965.

[13] Bellman, R. and Wing, G.M. : An introduction to Invariant Imbedding, Wiley, New York, 1975.

[14] Bickley, W.G. : Piecewise cubic interpolation and two point boundary value problems, Comp.J., 11(1968), 206-212.

[15] Boland, W.R. and Nelson, P. : Critical lengths by numerical integration of the associated Ricatti's equation to singularity, A.M.C., 1(1975), 67-82.

[16] Brabston, D.C. and Keller, H.B. : A numerical method for Singular two point boundary value problems, SIAM. J. Numr. Anal., 14(1977), 779-791.

[17] Bulirsch, R. Stoer, J., Deuflhard, P. : Numerical solution of nonlinear two point boundary value problems I. Numer. Math. Handbook series approximations, 1978.

[18] Carlde Boor : Practical guide to Splines, Springer Verlag, Berlin, Heidelberg, 1976.

[19] Casti, J. and Kalaba : Imbedding Methods in Applied Mathematics, Addi-Wes Pub. Comp. 1973.

[20] Chandrasekar, S. : Stability of steller potential problem. Jl.Math.Phy. 24(1959), 1012-1016.

[21] Chawla, M.M. : Finite Difference Methods and their convergence for a class of singular two point boundary value problems. Numer.Math, 39(1982), 341-350.

[22] Cho, S.M. and Sunderland, J.E. : Phase change problems with temperature dependent thermal conductivity, Jl. Heat transfer, ASME, 96 (1974), 214-217.

[23] Ciarlet, P.G. Natterer, F. and Varga, R.S. : Numerical methods of high order accuracy for nonlinear boundary value problem I. One dimensional problems, Numer.Math., 9(1967), 394-430.

[24] Ciarlet, P.G. Schult, M.M. and Varga, R.S. : Numerical methods of high order accuracy for singular non-linear boundary value problems. Numer. Math., 15(1970), 87-99.

[25] Coddington, E.A. and Levinson, N. : Theory of ordinary differential equations'. McGraw-Hill, New York 1955.

[26] Cohen A.M. and Jones, D. : A note on the numerical solution of some singular second order differential equations, Jl. Inst. Math.Applics.13(1974), 379-384.

[27] Collatz, L. : The numerical treatment of Differential equations Springer Verleg, Berlin, 1960.

[28] Daniel, J.W. and Swartz, B. : Extrapolated collocation for two point boundary value problems using cubic splines, Los Alamos Scientific Laboratory, Report LA-DC-72-1520, 1972.

[29] DeHoog, F.R. and Weiss, R. : Difference methods for boundary value problems with a singularity of the first kind, SIAM. Jl. Numer. Anal., 13(1976), 775-813.

[30] ——— : Collocation methods for singular boundary value problems, SIAM Jl. Num. Anal.15(1978), 198-217.

[31] ——— : The numerical solution of boundary value problems with an essential singularity, SIAM Jl. Num. Anal.16(1979), 637-669.

[32] ——— : The numerical solution of boundary value problems on infinite interval, Computing, 9(1980).

[33] Denman, E. : Invariant imbedding and linear systems in Invariant imbedding, Springer-Verleg, Berlin, Heidelberg, New York,1971.

[34] Denman,E. and Mingle,D. : Invariant imbedding to non-uniform elastic problem. Jl.Comp.Phys. 27(1971),771-776.

[35] Deodell,E.J. : The construction of finite difference approximation to ordinary differential equations, SIAM. Jl. Num. Anal. 15(1978), 450-465.

[36] [illegible] : Finite difference methods for non-singular boundary problems, SIAM. Jl.Num.Anal. 16(1979),173-189.

[37] Deodell,E.J. and Reddien,G.W. : Finite difference methods for singular two point boundary value problems, SIAM. Jl.Num.Anal.,21(1984), 300-313.

[38] Elder,I.T. : An invariant imbedding method for computation of eigenlengths of singular two point boundary value problems, Jl. Math. Anal. Applics, 85(1982),360-384.

[39] Eriksson,K. and Thomee Vidor : Galerkin methods for Singular boundary value problems in one space dimension, Math.Comp. 42(1984),345-367.

[40] Fehlberg,E. : Classical fifth-sixth seventh and eighth order Runga-Kutta formulas with step size control . NASA Technical Report, NASA TR R-287, 1968.

[41] Forsyth, G.E. Melcom, M.A. and Cleve,B.M. : Computer methods for Mathematical Computation, Prentice Hall Inc. 1977.

[42] Fox,L. : The numerical solution of two point boundary value problems in ordinary differential equations, Oxford University,1957.

[44] Fox, L. and Parker, I.B. : Chebyshev Polynomials in Numerical Analysis Oxford University Press, 1972.

[45] Fyfe, D.J. : The use of cubic splines in the solution of two point boundary value problems, Comp. Jl. 12(1969) 188-192.

[46] Grosch, G.E. and Orszag, S.A. : Numerical solution of problems in unbounded regions by coordinate transformation. Jl.Comp. Physics, 25(1977) 273-296.

[47] Gustaffsson, B. : A numerical method for solving singular boundary value problems, Numer. Math., 21(1973) 328-344.

[48] Hlavacek, V., Marck, M. and Kabicrk, M. : Modelling of chemical reactions- X Chem.Engg.Sci. 23(1968) 1083-1097.

[49] Holt, J.F. : Numerical solution of nonlinear two point boundary value problems by finite difference methods, Comm.ACM, 7(1964) 363-373.

[50] Jamet, P. : On the conversatsion of inite difference approximation to one dimensional singular boundary value problems, Numer.Math. 14(1970), 355-378.

[51] Jesperson, P. : Ritz-Galerkin Methods for singular two point boundary value problems, SIAM. Jl. Numer.Anal. 15(1978), 813-834.

[52] Kalaba, R. : Dynamic programming and the variational principles of classical and statistical mechanics, in developments in Mechanics Vol.1, Plenum Press, New York, 1961.

[53] Kalaba, R. and Kagiwada, H.H. : A New Initial-Value Method for Internal Intensities in Radiative Transfer, The Astrphys. J. 147 (1967), 301-309.

[44] Fox,L. and Parker,I.B. : **Chebyshev** Polynomials in Numerical Analysis Oxford University Press,1972.

[45] **Fyfe**,D.J. : The use of cubic splines in the solution of two point boundary value problems, Comp. Jl. 12(1969) 188-192.

[46] Grosch,G.E. and Orszag,S.A. : Numerical solution of problems in unbounded regions by coordinate transformation. Jl.Comp. Physics,25(1977) 273-296.

[47] Gustaffsson,B. : A numerical method for solving singular boundary value problems, Numer. Math.,21(1973) 328-344.

[48] **Hlavacek**, V., Marck,M. and Kabicrk,M. : Modelling of chemical reactions- X Chem.Engg.Sci.23(1968) 1083-1097.

[49] Holt,J.F. : Numerical solution of nonlinear two point boundary value problems by finite difference methods, Comm.ACM, 7(1964) 363-373.

[50] Jamet,P. : On the conversat**sion of** inite difference approximation to one dimensional singular boundary value problems, Numer.Math.14(1970), 355-378.

[51] Jesperson,P. : Ritz-Galerkin Methods for singular two point boundary value problems, SIAM. Jl. Numer.Anal.15(1978),813-834.

[52] Kalaba, R. : Dynamic programming and the variational principles of classical and statistical mechanics, in developments in Mechanics Vol.1,Plenum Press, New York,1961.

[53] Kalaba, R. and Kagiwada,H.H. : A New Initial-Value Method for Internal Intensities in Radiative Transfer, The Astrphys. J. 147 (1967), 301-309.

[54] Keller, H.B. : Numerical solution of boundary value problems for ordinary differential equation. Survey and some recent results on difference methods in numerical solutions of boundary value problems for ordinary differential equations. (Ed. A.K.Aziz). Academic Press, New York 1975, 27-88.

[55] ________ : Numercial methods for two point boundary value problems, London, Blaisdell 1968.

[56] ________ : Numercial solution of two point boundary value problems CBMS-NSF Regional Conf. Series in Applied Maths. 24, SIAM, Philadelphia 1976.

[57] ________ : Accurate Difference Methods for linear ordinary differential systems subject to linear constraints, SIAM Jl. Num. Anal, 6(1969), 8-30.

[58] Keller, H.B., and Lentini, M. : Invariant imbedding, the box scheme an equivalence between them. SIAM, Jl. Num. Anal, 19(1982), 942-962.

[59] Krishnamoorthy, E.V. : Computational based Numerical Algorithms. East-West Press, 1976.

[60] Lentini, M. : Numerical solution of the beam equation with non uniform foundation coefficient, Jl. of Appl. Mechanics, 46(1978), 901-904.

[61] Lentini, M., and Keller, H.B. : The Von-Karman Swirling Slows, SIAM Jl. Num. Anal., 38(1980), 52-64.

[62] ________ : Boundary value problems over semi infinite intervals and their numerical solution. SIAM Jl. Num. Anal., 17(1980 a), 557-604.

[63] Lentini, M. and Pereyra, Y. : An adaptive finite difference solver for non linear two point boundary value problems with mild boundary layers, SIAM Jl. Numer. Anal, 14(1977), 91-111.

[64] Markowich , P.A. : A Theory for the approximation of solutions of boundary value problems on infinite intervals, SIAM. Jl. Num. Anal, 13(1982), 721-727.

[65] ——— : Collocation Method for ''long'' interval problems, Math. Comput., 40 (1983), 123-150.

[66] Meyer, G.H. : Initial value methods for boundary value problems, theory and application of invariant imbedding. Academic press, New York and London, 1973.

[67] Na, T.Y. : Computational Methods in Engineering and boundary value problems, Academic press, New York, 1979.

[68] Natterer, F. : A generalised spline method for singular boundary value problems of ordinary differential equations, Line. Alge. Applics, 7, (1973), 189-216.

[69] Nelson, P. and Scott, M.R. : Interval values in particle transport by the method of invariant imbedding, Jl. Math. Appl. Applics, 34(1971), 628-643.

[70] Nelson, P. and Elder, T. : Calculation of eigenfunction for the context of integration-to-blowup, SIAM Jl. Num. Anal. 14(1977) 124-136.

[71] Nelson, P., Sagong, S, and Elder, T. : Invariant imbedding applied to Homogenuous two point boundary value problems with a singularity of first kind, Appl. Math. Comput. 9(1981), 93-110.

[72] Parter, V. : Numerical methods for generalized axially symmetric potentials. SIAM. Journal, series B2, (1965) 500-516.

[73] Reddien, G.W., and Schumaker, L.L. : On a collocation method for singular two point boundary value problems, Numer. Math, 25(1976), 433-456.

[74] Reddien, G.W. : Projection methods and singular two point boundary value problem, Numer. Math., 21(1973), 193-2o3.

[75] Rentrop, P. : A Tayler series method for the numerical solution of two point boundary value problems, Numer. Math. 31(1979), 359-375.

[76] ________ : Numerical solution for singular Ginzburg-Landau equations by Mulliple shooting computing, 16(1976), 61- 67.

[77] Roberts, S.M. : Reduction and the Kagiwada Kalaba Method of invariant imbedding, Jl. Math. Anal. Applics, 72(1979), 615-628.

[78] Roberts, S.M., and Shipman, J.S. : Two point boundary value problems, Shooting Methods. American Elsevier, New York 1972.

[79] ________ : A new motivation for the Scott's formulation of invariant imbedding, Jl. Math. Anal. Applics 64(1978), 480-487.

[80] Robertson, T. : Linear two point boundary value problems on infinite intervals, Math. Compt, 25(1972), 470-481.

[81] Rose, M.E. : Finite difference for solutions for differential equations, Math. Comp. 18(1964), 179-195.

[82] Russell and Shampine, L.F. : A collocation method for boundary value problems, Numer. Math. 19(1972), 1-28.

[83] ________ : Numerical methods for singular boundary value problems. SIAM. Jl. Num. Anal, 12(1975), 13-36.

[84] Schneider, W. : A similarity solution for combined forced and free convection flow over a horizontal plate, Int. Jl. Heat and Mass Transfer, 23(1979), 1401-1406.

[85] Scott, M.R. : Invariant imbedding and its application to ordinary differential equations. Appl. Math and computation. No.1, Addison-Wesley, Publishing Comp, Mass. London, Amsterdam 1973.

[86] ________ : Numerical solution of unstable initial value problems by invariant imbedding, Comput. Jl, 13(1970) 397-400.

[87] ________ : On the conversion of boundary value problems into stable initial value problem via several imbedding algorithms. Numerical solution of ordinary differential equations edited by A.K.Aziz.

[88] ________ : Invariant imbedding and the calculation of interval values, Jl. Math.Anal. Applics 28(1969), 112-115.

[89] Scott, M.R., Shampine, L.F., and Wing, G.M. : Invariant imbedding and the calculation of eigenvalues for strum-Liouville systems Computing, 4(1969) 10-23.

[90] Shoemaker, E.M. : Invariant imbedding applied to eigenvalue problems in Mechanics, Jl. Appl. Mech., 32(1965).

[91] Weinitschke, H.J. : On the stability, problem for shallow spherical shells, Jl. Math. Phy. 38(1958), 209-231.

[92] Weinmüller, E. : Difference methods for singular boundary value problem of second order, Tech. Report. 1984.

[93] ____________, __ : On the boundary value problem for systems of ordinary differential equations with a singularity of first kind. SIAM. Jl. Math. Anal 15(1984), 287-307.

APPENDIX – A

LIST OF PROGRAM FOR CHAPTER – III

APPENDIX - III
****

```
MAIN PROGRAM
CONTINUOUS IMBEDDING FOR SINGULAR
BOUNDARY VALUE PROBLEMS.
*****************************************************
                  Y''(X)+F1(X)*Y'(X)+F2(X)*Y(X)=F3(X)
                       Y(Xo)=ALPHA ; Y(b)=BETA .
*****************************************************
F1, F2 AND F3 -- THE COEFF.FUNCTIONS FROM THE GIVEN EQN.
ALPHA AND BETA -- GIVEN ARBITARY CONSTANTS
X - CORRESPONDS THE VALUE OF DELTA.
M1 AND M2 -- ROOTS OF THE INDICIAL EQUATION.
N1 - NUMBER OF THE TERMS IN THE SERIES EXPANSION.
A10,A1(I), I=1,2 .....N1 AND B10,B1(I) I=1,2...N1
C10,C1(I), I=1,2....N2 AND D10,D1(I), I=1,2...N1
ARE THE CONSTANTS IN THE SERIES SOLUTION.
R1,R2,DR1 AND DR2 -- CALCULATED BY USING THE
                        SERIES SOLUTION.
DR1 AND DR2 -- THE FIRST AND SECOND DERIVATIVES
                  OF THE SERIES EXPANSIONS.
AONE =A, BONE =B AND CONE =C -- COEFF.FROM THE BOUNDARY
CONDITION AT DELTA
-----------------------------------------------------
EXTERNAL ALL
REAL Z,Y(4),ZOUT,RELERR,ABSERR,K11,K22,K33,K44,
1                                 K55,K66,K77
REAL ZFINAL,ZPRINT,WORK(39)
INTEGER IWORK(5),IFLAG,NEQN
```

```
------------------------------------------------------------
DIMENSION X1(100,100),U(100),V(100),A1(100),B1(100)
DIMENSION C1(100),D1(100)
------------------------------------------------------------
REAL M1,M2
OPEN(UNIT=13,DEVICE='DSK',FILE='SUM1.DAT')
READ(13,*)N1,M1,M2,X
READ(13,*)A10,(A1(I), I=1,N1)
READ(13,*),B10,(B1(I), I=1,N1)
READ(13,*)C10,(C1(I), I=1,N1)
READ(13,*)D10,(D1(I), I=1,N1)

S11=A1(N1)
DO 11 I=1,N1
N2=N1+1-I
S11=S11*X+A1(N2)
S11=S11*X+A10

DS11=B1(N1)
DO 12 I=2,N1
N3=N1+1-I
DS11=DS11*X+B1(N3)
DS11=DS11*X+B10

S22=C1(N1)
DO 14 I=2,N1
N4=N1+1-I
S22=S22*X+C1(N4)
S22=S22*X+C10
```

```
DS22=D1(M1)
DO 15 I=2,M1
N5=M1+1-I
DS22=DS22*X+D1(N5)
DS22=DS22*X+D10
TYPE*,S11,DS11,S22,DS22
------------------------------------------------------------
R1=X**M1*S11
DR1=M1*X**(M1-1)*S11+X**M1*DS11
R2=X**M2*S22
DR2=M2*X**(M2-1)*S22+X**M2*DS22
TYPE*,R1,DR1,R2,DR2
AONE=DR2
BONE=-R2
CONE=R1*DR2-DR1*R2
TYPE*,AONE,BONE,CONE
------------------------------------------------------------
-------------------------------------------------------
SAMPLE PROBLEM :3.1
Y(X)=U(X); Y'(X)U'(X)=V(X).
------------------------------------------------------
Z -CORRESPONDS TO X WHICH IS DELTA TO BE GIVEN.
Z=0.5
J=1
NUMBER OF EQUATIONS AND INITIAL CONDITIONS.
NEQN=6
Y(1)=0.0
Y(2)=1.0
Y(3)=0.0
Y(4)=1.0
```

```
Y(5)=0.0
Y(6)=0.0
-------------------------------------------------------
RELERR=1.0E-5
ABSERR=0.0
ZFINAL=1.0
ZPRINT=0.1
IFLAG=1
ZOUT=Z
CALL RKF45(ALL,NEQN,Y,Z,ZOUT,RELERR,ABSERR,
1           IFLAG,WORK,IWORK)
TYPE*,J,Z,Y(1),Y(2),Y(3),Y(4),Y(5),Y(6)
GO TO(80,20,30,40,50,60,70,80),IFLAG
ZOUT=Z+ZPRINT
DO 111 I=1,NEQN
Y1(J,I)=Y(I)
J=J+1
IF(Z.LT.ZFINAL)GO TO 10
SOLVE THE SYSTEM OF SIMULTANUOUS EQUATIONS.
K11=UL-Y(3)
VDELTA=((K11*Y(4)+Y(1)*Y(6))*AONE-CONE*(Y(4)*Y(2)-Y(5)*Y(1)))/
1   (Y(1)*AONE-((Y(4)*Y(2)-Y(5)*Y(1))*BONE))
UDELTA=(CONE-BONE*VDELTA)/AONE
TYPE*,UDELTA,VDELTA,VDELTA
-------------------------------------------------------
U(1)=UDELTA
V(1)=VDELTA
U(J-1)=UL
SOLUTION IN TERMS OF U(1)'S.
DO 551 I=2,J-2
```

```
V(I)=(VDELTA-Y1(I,5)*UDELTA-Y1(I,6))/Y1(I,4)
U(I)=Y1(I,1)*V(I)+Y1(I,2)*UDELTA+Y1(I,3)
TYPE*,U(I),V(I)
CONTINUE
TYPE 232
FORMAT(5X,'-----------------------------------------------'/)
TYPE 235
FORMAT(8X, 'INVARIANT IMBEDDING SOLUTION'/)
TYPE 236
FORMAT(5X,'-----------------------------------------------'/)
DO 555 I=1,J-1
TYPE 233,U(I),V(I)
FORMAT(5X,E20.10,5X,E20.10/)
CONTINUE
TYPE 237
FORMAT(5X,'-----------------------------------------------')
STOP
TYPE 31,RELERR,ABSERR
GO TO 10
GO TO 10
ABSERR=1.0E-13
TYPE 31,RELERR,ABSERR
GO TO 10
RELERR=10.0*RELERR
TYPE 31,RELERR,ABSERR
IFLAG=2
GO TO 10
TYPE 71
IFLAG=2
GO TO 10
```

```
      TYPE 81
      FORMAT(2X,'TOLERANCES RESET',5X,2E12.3)
      FORMAT(5X,'MUCH OUTPUT')
      FORMAT(5X,'IMPROPER CALL')
      STOP
      END
```

SUBROUTINES ARE ALL, RKF45, RKFS, FEHL:-

RKF45 - Fehlberg Fourth-Fifth Order
Runge-Kutta Method.
REFERENCES :
E.FEHLBERG, LOW-ORDER CLASSICAL RUNGE
KUTTA FORMULA STEPSIZE CONTROL, NASA
TR-R315.
L.F.SHAMPINE, H.A.WATTS.
SANDIA LABORATORIES REPORT SAND 76-0585.

FOR THE TEST EXAMPLE 3.1 THE CORRESPONDING INITIAL
VALUE PROBLEMS ARE GIVEN.
YP(1) -- S1'(X) ,YP(2) -- S2'(X), YP(3) -- S3'(X),
YP(4) -- Q1'(X), YP(5) -- Q2'(X), YP(6) -- Q3'(X).

```
      SUBROUTINE ALL(Z,Y,YP)
      REAL Z,Y(4),YP(4)
      YP(1)=1.0+(0.5/Z)*Y(1)-(Y(1)*Y(1))
      YP(2)=-Y(1)*Y(2)
      YP(3)=-Y(1)*Y(3)
      YP(4)=((0.5/Z)-Y(1))*Y(4)
      YP(5)=-Y(4)*Y(2)
```

```
      YP(6)=-Y(3)*Y(4)
      RETURN
      END
-----------------------------------------------------------------
      SUBROUTINE RKF45(F,NEQN,Y,Z,ZOUT,RELERR,ABSERR,IFLAG,
     1WORK,IWORK)
      INTEGER NEQN,IFLAG,IWORK(5)
      REAL Y(NEQN),Z,ZOUT,RELERR,ABSERR,WORK(1)
      EXTERNAL F
      KIM=NEQN+1
      K1=KIM+1
      K2=K1+NEQN
      K3=K2+NEQN
      K4=K3+NEQN
      K5=K4+NEQN
      K6=K5+NEQN
      CALL RKFS(F,NEQN,Y,Z,ZOUT,RELERR,ABSERR,IFLAG,WORK(1),
     1WORK(KIM),WORK(K1),WORK(K2),WORK(K3),WORK(K4),WORK(K5),
     2WORK(K6),WORK(K6+1),IWORK(1),IWORK(2),IWORK(3),IWORK(4),
     3IWORK(5))
      RETURN
      END
-----------------------------------------------------------------
      SUBROUTINE RKFS(F,NEQN,Y,Z,ZOUT,RELERR,ABSERR,IFLAG,YP,H,
     4F1,F2,F3,F4,F5,SAVRE,SAVAE,NFE,KOP,INIT,JFLAG,KFLAG)
      LOGICAL HFAILD,OUTPUT
      INTEGER NEQN,IFLAG,NFE,KOP,INIT,JFLAG,KFLAG
      REAL Y(NEQN),Z,ZOUT,RELERR,ABSERR,H,YP(NEQN)
      REAL F1(NEQN),F2(NEQN),F3(NEQN),F4(NEQN),F5(NEQN),SAVRE,SAVAE
      REAL A,AE,DT,EE,EEOET,ESTTOL,ET,HMIN,REMIN,RER,S,SCALE,
```

```
1TOL,TOLL,U26,EPSP1,EPS,YPK
EXTERNAL F
INTEGER K,MAXNFE,MFLAG
REAL AMAX1,AMIN1
DATA REMIN/1.0E-6/
DATA MAXFNE/3000/
IF(NEQN.LT.1)GO TO 10
IF((RELERR.LT.0.0).OR.(ABSERR.LT.0.0))GO TO 10
MFLAG=IABS(IFLAG)
IF((MFLAG.EQ.0).OR.(MFLAG.GT.8))GO TO 10
IF(MFLAG.NE.1)GO TO 20
EPS=1.0
EPS=EPS/2.0
EPSP1=EPS+1.0
IF(EPSP1.GT.1) GO TO 5
U26=26.0*EPS
GO TO 50
IFLAG=8
RETURN
IF((Z.EQ.ZOUT).AND.(KFLAG.NE.3))GO TO 10
IF(MFLAG.NE.2)GO TO 25
IF((KFLAG.EQ.3).OR.(INIT.EQ.0))GO TO 45
IF(KFLAG.EQ.4)GO TO 40
IF((KFLAG.EQ.5).AND.(ABSERR.EQ.0.0))GO TO 30
IF((KFLAG.EQ.6).AND.(RELERR.LE.SAVRE).AND.
1(ABSERR.LE.SAVAE))GO TO 30
GO TO 50
IF(IFLAG.EQ.3)GO TO 45
IF(IFLAG.EQ.4)GO TO 40
IF((IFLAG.EQ.5).AND.(ABSERR.GT.0.0))GO TO 45
```

```
STOP
NFE=0
IF(MFLAG.EQ.2)GO TO 50
IFLAG=JFLAG
IF(KFLAG.EQ.3)MFLAG=IABS(IFLAG)
JFLAG=IFLAG
KFLAG=0
SAVRE=RELERR
SAVAE=ABSERR
RER=2.0*EPS+REMIN
IF(RELERR.GE.RER)GO TO 55
IFLAG=3
KFLAG=3
RETURN
DT=(ZOUT-Z)
IF(MFLAG.EQ.1)GO TO 60
IF(INIT.EQ.0)GO TO 65
GO TO 80
INIT=0
KOP=0
A=Z
CALL F(A,Y,YP)
NFE=1
IF(Z.NE.ZOUT)GO TO 65
IFLAG=2
RETURN
INIT=1
H=(ABS(DT))
TOLN=0.
DO 70 K=1,NEQN
```

```
      TOL=RELERR*ABS(Y(K))+ABSERR
      IF(TOL.EQ.0)GO TO 70
      TOLN=TOL
      YPK=ABS(YP(K))
      IF(YPK*H**5.GT.TOL)H=(TOL/YPK)**0.2
0     CONTINUE
      IF(TOLN.LE.0.0)H=0.0
      H=AMAX1(H,U26*AMAX1(ABS(Z),ABS(DT)))
      JFLAG=ISIGN(2,IFLAG)
      H=SIGN(H,DT)
      IF(ABS(H).GE.2.0*ABS(DT))KOP=KOP+1
      IF(KOP.NE.100)GO TO 85
      KOP=0
      IFLAG=7
      RETURN
5     IF(ABS(DT).GT.U26*ABS(Z))GO TO 95
      DO 90 K=1,NEQN
      Y(K)=Y(K)+DT*YP(K)
      A=ZOUT
      CALL F(A,Y,YP)
      NFE=NFE+1
      GO TO 300
      OUTPUT=.FALSE.
      SCALE=2.0/RELERR
      AE=SCALE*ABSERR
0     HFAILD=.FALSE.
      HMIN=U26*ABS(Z)
      DT=ZOUT-Z
      IF(ABS(DT).GE.2.0*ABS(H))GO TO 200
      IF(ABS(DT).GT.ABS(H))GO TO 150
```

```
OUTPUT=.TRUE.
H=DT
GO TO 200
H=0.5*DT
IF(NFE.LE.MAXFNE)GO TO 220
IFLAG=4
KFLAG=4
RETURN
CALL FEHL(F,NEON,Y,Z,H,YP,F1,F2,F3,F4,F5,F1)
NFE=NFE+5
EEOET=0.0
DO 250 K=1,NEON
ET=ABS(Y(K))+ABS(F1(K))+AE
IF(ET.GT.0.0)GO TO 240
IFLAG=5
RETURN
EE=ABS((-2090.0*YP(K)+(21970.0*F3(K)-15048.0*F4(K)))+
1(22528.0*F2(K)-27360.0*F5(K)))
EEOET=AMAX1(EEOET,EE/ET)
ESTTOL=ABS(H)*EEOET*SCALE/752400.0
IF(ESTTOL.LE.1.0)GO TO 260
HFAILD=.TRUE.
OUTPUT=.FALSE.
S=0.1
IF(ESTTOL.LT.59049.0)S=0.9/ESTTOL**0.2
H=S*H
IF(ABS(H).GT.HMIN)GO TO 200
IFLAG=6
KFLAG=6
RETURN
```

```
Z=Z+H
DO 270 K=1,NEON
Y(K)=F1(K)
A=Z
CALL F(A,Y,YP)
NFE=NFE+1
S=5.0
IF(ESTTOL.GT.1.889568E-4)S=0.9/ESTTOL**0.2
IF(HFAILD)S=AMIN1(S,1.0)
H=SIGN(AMAX1(S*ABS(H),HMIN),H)
IF(OUTPUT)GO TO 300
IF(IFLAG.GT.0)GO TO 100
IFLAG=-2
RETURN
Z=ZOUT
IFLAG=2
RETURN
END
SUBROUTINE FEHL(F,NEON,Y,Z,H,YP,F1,F2,F3,F4,F5,S)
INTEGER NEON
REAL Y(NEON),Z,H,YP(NEON),F1(NEON),F2(NEON),
1F3(NEON),F4(NEON),F5(NEON),S(NEON)
REAL CH
INTEGER K
CH=H/4.0
DO 221 K=1,EQN
F5(K)=Y(K)+CH*YP(K)
CALL F(Z+CH,F5,F1)
CH=3.0*H/32.0
DO 222 K=1,NEON
```

```
F5(K)=Y(K)+CH*(YP(K)+3.0*F1(K))
CALL F(Z+3.0*H/8.0,F5,F2)
CH=H/2197.0
DO 223 K=1,NEON
F5(K)=Y(K)+CH*(1932.0*YP(K)+(7296.0*F2(K)-7200.0*F1(K)))
CALL F(Z+12.0*H/13.0,F5,F3)
CH=H/4104.0
DO 224 K=1,NEON
F5(K)=Y(K)+CH*((8341.0*YP(K)-845.0*F3(K))+(29440.0*F2(K)-
132832.0*F1(K)))
CALL F(Z+H,F5,F4)
CH=H/20520.0
DO 225 K=1,NEON
F1(K)=Y(K)+CH*((-6080.0*YP(K)+(9295.0*F3(K)-5643.0*F4(K)))
1+(41040.0*F1(K)-28352.0*F2(K)))
CALLF(Z+H/2.0,F1,F5)
CH=H/7618050.0
DO 230 K=1,NEON
S(K)=Y(K)+CH*((902880.0*YP(K)+(3855735.0*F3(K)-1371249.0*
1F4(K)))+(3953664.0*F2(K)+277020.0*F5(K)))
RETURN
END
```

APPENDIX - B

LIST OF PROGRAM FOR CHAPTER - V

APPENDIX - V

****

MAIN PROGRAM

FOURTH PORDER FINITE DIFFERENCE TECHNIQUE.

```
          Y''(X)+(P1(X))*Y'(X)-Q(X)*Y(X)=F(X)
                 Y'(0)=0 ; Y(1)=BETA.
          WHERE P1(X)=K/X .
```

ARGUMENTS

****

N1 - NUMBER OF MESH POINTS.

H - STEP SIZE

P1, Q AND F -- THE COFF.FUNCTIONS FROM THE GIVEN EQUATION.

DP11 AND DDP11 -- THE FIRST AND SECOND DERIAVATIVES OF P1.

DQ AND DDQ -- THE FIRST AND SECOND DERIAVATIVES OF Q

DR AND DDR -- THE FIRST AND SECOND DERIAVATIVES OF R

M1 -- MESH PONT WHERE THE SOLUTION TO BE OBTAINED.

HERE THE INITIAL CONDITION TO BE GIVEN

```
BETA=5.5
--------------------------------------------------------
DIMENSION X1(0:100),X2(0:100),X3(0:100),Y1(0:100),Y2(0:100),
1         Y3(0:100),Z1(0:100),Z2(0:100),Z3(0:100),L(0:100),
1         W(0:100),T(0:100),M(0:100),N(0:100),
1         P(0:100),U(0:100),V(0:100),Y(0:100)
REAL M,N,L
*************************************************************
```

```
OPEN(UNIT=10,DEVICE='DSK',FILE='FD.DAT')
READ(10,*)N1,K,M1
H=1./FLOAT(N1)
Y1(0)=R(0)/(1+K)
Y2(0)=DR(0)/(1+K)
Y3(0)=DDR(0)/(1+K)
Z1(0)=F(0)/(1+K)
Z2(0)=DF(0)/(1+K)
Z3(0)=DDF(0)/(1+K)
-------------------------------------------------------------
M(0)=2.0+((H**2)/6)*(5.0*Y1(0))+((H**4)/12)*Y3(0)
L(0)=1.0-((H**2)/12)*Y1(0)-((H**3)/24)*(2.0*Y2(0))
N(0)=1.0-(((H**2)/12)*Y1(0))+((H**3)/24)*(2.0*Y2(0))
P(0)=(H**2)*Z1(0)+((H**4)/12)*Z3(0)
-------------------------------------------------------------
DO 111 I=1,M1
AI=X+I*H
X1(I)=P1(AI)
X2(I)=DP1(AI)
X3(I)=DDP1(AI)
Y1(I)=R(AI)
Y2(I)=DR(AI)
Y3(I)=DDR(AI)
Z1(I)=F(AI)
Z2(I)=DF(AI)
Z3(I)=DDF(AI)
CONTINUE
DO 20 I=1,N1-1
M(I)=2.0+((H**2)/6)*(5.0*Y1(I)+X1(I)*X1(I)+X2(I))+
1       ((H**4)/12)*(Y3(I)+X1(I)*Y2(I)-X2(I)*Y1(I))
```

```
L(I)=1.0+(H/2)*X1(I)+((H**2)/12)*(X1(I)*X1(I)+X2(I)-Y1(I))+
1        ((H**3)/24)*(X3(I)-2.0*Y2(I)-X1(I)*Y1(I))
N(I)=1.0-(H/2)*X1(I)+((H**2)/12)*(X1(I)*X1(I)+X2(I)-Y1(I))-
1        ((H**3)/24)*(X3(I)-2.0*Y2(I)-X1(I)*Y1(I))
P(I)=(H**2)*Z1(I)+((H**4)/12)*(Z3(I)+X1(I)*Z2(I)-X2(I)*Z1(I))
CONTINUE
-------------------------------------------------------
THE INITIAL CONDITIONS  FOR W'S AND T'S
W(0)=(L(0)+N(0))/M(0)
T(0)=-P(0)/M(0)
-------------------------------------------------------
DO 30 I=1,N1-1
W(I)=(L(I))/(M(I)-N(I)*W(I-1))
T(I)=(P(I)-N(I)*T(I-1))/(N(I)*W(I-1)-M(I))
CONTINUE
-------------------------------------------------------
Y(N1)=BETA
DO 40 I=N1-1,0,-1
Y(I)=W(I)*Y(I+1)+T(I)
CONTINUE
-------------------------------------------------------
TYPE 900
FORMAT(5X,'------------------------------------'/)
DO 45 I=0,N1,M1
TYPE 901,Y(I)
FORMAT(5X,E20.10/)
CONTINUE
TYPE 902
FORMAT(5X,'------------------------------------')
GO TO 211
```

```
STOP
END
------------------------------------------------------------
SAMPLE PROGRAM
PROBLEM 5.1
------------------------------------------------------
REAL FUNCTION P1(X)
P1=2.0/X
RETURN
END
REAL FUNCTION R(X)
R=4.0
RETURN
END
REAL FUNCTION F(X)
F=-2.0
RETURN
END
REAL FUNCTION DP1(X)
DP1=-2.0/X**2
RETURN
END
REAL FUNCTION DR(X)
DR=0.0
RETURN
END
REAL FUNCTION DF(X)
DF=0.0
RETURN
```

```
END
REAL FUNCTION DDP1(X)
DDP1=4.0/(X**3)
RETURN
END
REAL FUNCTION DDR(X)
DDR=0.0
RETURN
END
REAL FUNCTION DDF(X)
DDF=0.0
RETURN
END
```

APPENDIX - C

LIST OF PROGRAM FOR CHAPTER - VIII

APPENDIX - VIII

****

```
-------------------------------------------------------------------
MAIN PROGRAM
CUBIC SPLINE METHOD FOR
INFINITE INTERVAL PROBLEMS.
*****************************************************
        Y''(X)+P(X)*Y'(X)+Q(X)*Y(X)=R(X)
                Y(a)=alpha ; Y(INF)=BETA
        WHERE INF DENOTES THE INFINITY.
*****************************************************
P, Q AND R - THE FUNCTIONS FROM THE
GIVEN EQUATION
H - STEP SIZE
XINF =N - THE FINITE POINT
APZERO -ALPHA ZERO , BEZERO -  BETA ZERO,
AND K ARE THE CONSTANTS EVALUATED FROM
THE ASYMPTOTIC BOUNDARY CONDITIONS
M1 - THE MESH POINT WHERE THE SOLUTION
TO BE OBTAINED.
--------------------------------------------------------------
DOUBLE PRECISION A(0:2000),B(0:2000),C(0:2000),C1(0:2000),
1        E(0:2000),D(0:2000),T(0:2000),F(0:2000),
1        W(0:2000),Y(0:2000),X1(0:2000),
1        X2(0:2000),X3(0:2000),ALPH1,BETA1,GAMMA1,
1        APZERO,BEZERO,S2,S3,SS,SS1,TT,TT1,TT2,
1        UU,UU1,VV,VV1,YY,YY1
---------------------------------------------------------
OPEN (UNIT=15,DEVICE='DSK',FILE='CUB.DAT')
READ(15,*)N,H,APZERO,BEZERO,K,M1
```

```
      DO 21 I=0,N
      AI=X+I*H
      X1(I)=P(AI)
      X2(I)=Q(AI)
      X3(I)=R(AI)
      CONTINUE
      DO 20 I=1,N
      A(I)=(1.0-H*0.333333333*X1(I-1)+H*0.3333333*X1(I)-0.08333333*
     1        X1(I-1)*X1(I)*H*H)
      CONTINUE
      DO 30 I=1,N-1
      B(I)=(1.0-H*0.3333333*X1(I)+H*0.3333333*X1(I+1)-0.08333333*
     1        X1(I+1)*X1(I)*H*H)
      C1(I)=(1.0+0.2916666*H*(X1(I+1)-X1(I-1))-0.0833333*H*H*
     1        X1(I-1)*X1(I+1))
      TYPE*,A(I),B(I),C1(I)
      CONTINUE
      -----------------------------------------------------
      DO 40 I=1,N-1
      E(I)=(1.0+H*0.5*X1(I+1)+0.1666666*H*H*(X2(I+1)))*A(I)
      D(I)=(1.0-H*0.5*X1(I-1)+0.1666666*H*H*X2(I-1))*B(I)
      C(I)=(1.0+H*0.5*X1(I+1))*A(I)+(1.0-H*0.5*X1(I-1))*B(I)-
     1        (0.6666666*H*H*X2(I)*C1(I))
      F(I)=H*H*0.16666666*(A(I)*X3(I+1)+4.0*C1(I)*X3(I)+
     1        B(I)*X3(I-1))
      TYPE*,D(I),C(I),O(I)
      CONTINUE
-----------------------------------------------------------------
      TO FIND THE INITIAL CONDITIONS FOR W'S AND T'S
-----------------------------------------------------------------
```

```
SS=0.3333333*X1(N)-0.166666667*X1(N)*X1(N-1)+0.055555556*
1        H*H*X1(N)*X2(N-1)
SS1=(SS*APZERO)/A(N)
TT=0.083333333*H*X1(N)*X1(N-1)+0.16666667*X1(N-1)-0.16666667
1        *H*X2(N-1)-0.055555556*H*H*X1(N)*X2(N-1)
TT1=(TT*APZERO)/A(N)
TT2=-((SS1+TT1)-APZERO/H)
TYPE*,SS1,TT1,TT2
UU=0.111111111*H*H*X1(N-1)*X2(N)-0.33333333*X2(N)-0.3333337*
1        X1(N)+0.16666667*X1(N-1)+X1(N)
UU1=(UU*APZERO)/A(N)
VV=-(0.16666667*X1(N-1)+0.0833333333*H*X1(N)*X1(N-1)+
1        0.027777778*H*H*X1(N-1)*X2(N))
VV1=(VV*APZERO)/A(N)
YY=(UU1+VV1+APZERO/H+BEZERO)
TYPE*,UU1,VV1,YY
YY1=K+0.11111111*APZERO*H**2*X1(N-1)*X3(N)/B(N-1)-0.3333337*
1        APZERO*H*X3(N)/B(N-1)+0.05555556*APZERO*H**2*X1(N)*
1        X3(N-1)/B(N-1)-0.1666667*APZERO*H*X3(N-1)/A(N)-
1        0.05555556*X1(N)*X3(N-1)*APZERO**2/A(N)-0.027777778*
1        H**2*X1(N-1)*X3(N)/A(N)
TYPE*,YY1
----------------------------------------------------------
ALPH1=YY
BETA1=TT2
GAMMA1=YY1
----------------------------------------------------------
TO STORE THE VALUES OF W'S AND T'S BY USING
THE INITIAL VALUES OF W'S AND T'S
----------------------------------------------------------
```

```
W(N-1)=BETA1/ALPH1
DO 103 I=1,N-1
J1=N-I
J=J1-1
W(J)=D(J1)/(C(J1)-E(J1)*W(J1))
CONTINUE
T(N-1)=GAMMA1/ALPH1
DO 104 I=1,N-1
K1=N-I
K=K1-1
T(K)=(E(K1)*T(K1)-F(K1))/(C(K1)-E(K1)*W(K1))
CONTINUE
-----------------------------------------------------
HERE THE INITIAL CONDITION TO BE GIVEN.
Y(0)=1.0
--------------------------------------------------------
USING THE VALUES OF W(I)'S AND T(I)'S THE
SOLUTION Y(I)'S ARE CALCULATED BY FORWARD
PROCESS
---------------------------------------------------------
DO 90 I=0,N-1
Y(I+1)=W(I)*Y(I)+T(I)
TYPE*,I,Y(I)
CONTINUE
TYPE 210
FORMAT(12X,'----------------------'/)
TYPE 212
FORMAT(13X,'COMPUTED SOLUTION'/)
DO 100 I=0,N,N1
TYPE 213,Y(I)
```

```
FORMAT(10X,E20.10/)
CONTINUE
TYPE 214
FORMAT(12X,'----------------------')
GO TO 111
STOP
END
-------------------------------------------------------
SAMPLE PROGRAM
PROBLEM 8.1
-------------------------------------------------------
REAL FUNCTION P(X)
P=2.0
RETURN
END
REAL FUNCTION Q(X)
Q=-2.0
RETURN
END
REAL FUNCTION R(X)
R=-EXP(-2.0*X)
RETURN
END
-------------------------------------------------------
```

MATH-1984-D-RAM-NUM